

AFIT/DS/ENP/97-06

Kinetics and Spectroscopy of BrNO

DISSERTATION

Patrick Eugene Godfrey  
Captain, USAF

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# Kinetics and Spectroscopy of BrNO

## DISSERTATION

Presented to the Faculty of the School of Engineering  
of the Air Force Institute of Technology

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In Partial Fulfillment of the  
Requirements for the Degree of  
Doctor of Philosophy

Patrick Eugene Godfrey, B.S., M.S.  
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June, 1997

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## Kinetics and Spectroscopy of BrNO

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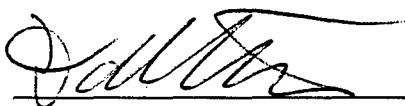
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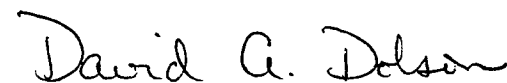
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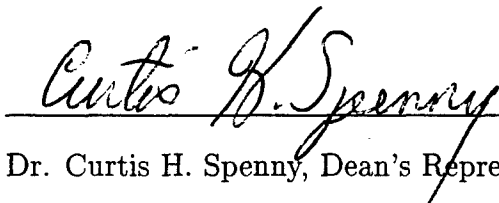
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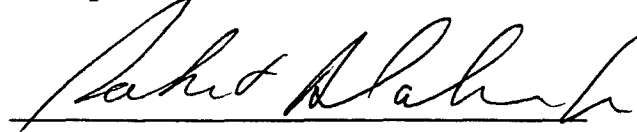
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Patrick Eugene Godfrey



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### *Abstract*

The infrared spectra and photochemistry of nitrosyl bromide, BrNO, are important to characterizing the performance of a recently demonstrated Br( $^2P_{1/2}$ )-NO( $v=2 \rightarrow v=1$ ) transfer laser pumped by photolysis of iodine molecules. This wavelength agile, mid-infrared laser may be a desirable source for remote sensing and infrared countermeasures missions. Nitrosyl bromide also plays a role in the destruction of stratospheric ozone.

The kinetics of BrNO formation and destruction were examined using time-resolved photolysis techniques. The equilibrium constant for the dark reaction  $\text{Br}_2 + 2\text{NO} \rightleftharpoons 2\text{BrNO}$  was determined as  $K_{\text{eq}} = 168 \pm 23 \text{ atm}^{-1}$  and the rate constant for the forward reaction as  $k_f = 1.40 \pm .18 \times 10^{-38} \text{ cm}^6/\text{molecule}^2\text{-s}$  at 293K. A novel technique for the fitting of the observed time profiles to the three-body kinetics was developed which utilizes the complete temporal profile to establish the rate coefficients.

When an equilibrium mixture of Br<sub>2</sub>, NO and BrNO is disturbed by photolysis, BrNO is rapidly removed by reaction with atomic bromine. For continuous photolysis, a new photostationary condition is achieved which shifts the equilibrium toward Br<sub>2</sub> and NO. A kinetic mechanism and rates for the photolysis of such mixtures has been validated for total pressures of 28-111 torr and nitric oxide to molecular bromine concentration ratios of 2.18-26.75, with an average Br<sub>2</sub> photolysis rate of 0.050 molecules/s.

The rotation structure of the  $\nu_1 + \nu_2 - \nu_3$ ,  $2\nu_1 - \nu_3$ ,  $2\nu_1$ ,  $3\nu_1$ ,  $2\nu_1 + \nu_3$  and  $3\nu_1 + \nu_3$  overtone and combination bands of BrNO were examined at high resolution ( $.005 - .01 \text{ cm}^{-1}$ ) using Fourier Transform Spectroscopy. Over 4900 spectral lines were recorded for the two isotopes  $^{79}\text{BrNO}$  and  $^{81}\text{BrNO}$ . The rotational and quartic distortion terms, inertia defects and asymmetry parameters were determined for

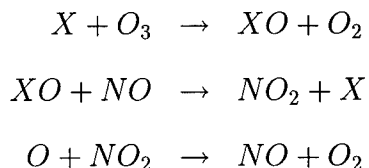
the (200), (300), (001), (200), (301) and (110) vibrational levels. The first-order vibration-rotation interaction terms were also determined.

# Kinetics and Spectroscopy of BrNO

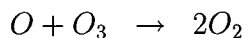
## *I. Introduction*

### *1.1 Motivation*

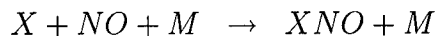
The research reported here focuses on nitrosyl bromide and was undertaken for two reasons. The first is that halogens have been linked to the chemical reactions believed to describe the ozone depletion cycle. Chlorofluorocarbons contain halogens that deplete ozone through the reactions:



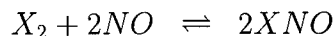
where X represents fluorine, chlorine, iodine or bromine. The net effect of these reactions is to reduce the ozone concentration:



The halogen atom is not consumed in these reactions but it may react with nitric oxide and a third body M to form a nitrosyl halide:



The halogen atoms may also form diatomic molecules that react with the NO, again creating nitrosyl halides:



If the halogen is present only as  $X_2$  or  $XNO$  molecules it cannot aid the depletion of ozone. Determining the effects of these processes requires a thorough understanding of the kinetics of the reactions. The first part of this research effort addressed some of the kinetic issues that arise when a halogen reacts with nitric oxide.

The Air Force's interest in photolytically-pumped chemical lasers also motivated this research. A requirement exists to develop kilowatt-class infrared lasers operating in the 3 to 5  $\mu\text{m}$  region of the spectrum for electro-optic countermeasures. Airborne operation imposes stringent requirements on candidate systems. The system must be energy-efficient because aircraft power supplies are limited. The ability to operate at a variety of wavelengths allows the system to counter different threats and makes counter-counter measures more difficult. Finally, the system must be able to operate despite the accelerations and vibrations it will experience when mounted to an aircraft. Unlike optically-pumped lasers, photolytically-pumped lasers do not need wavelength-stable light sources that mandate stable optical cavities. Instead, the pump can vary over a relatively broad wavelength range, making such lasers ideal for use in high-vibration environments. The necessary tunability can be achieved using Electronic  $\rightarrow$  Vibrational energy transfer from gas-phase, electronically-excited atoms to the ro-vibrational modes of a suitable molecular species.

One proposed system depends on E-V energy transfer from excited bromine atoms to  $\text{NO}(v=2)$  molecules. A complication involved in creating this system arises from the fact that  $\text{Br}_2$  and  $\text{NO}$  react to form  $\text{BrNO}$ . The formation of this molecule may limit system performance by depleting the populations of  $\text{NO}$  and  $\text{Br}(^2\text{P}_{1/2})$ . The kinetic studies reported here increase our understanding of the chemical reactions involved in the production and destruction of  $\text{BrNO}$ .

## 1.2 *Presentation*

This dissertation consists of two almost-independent parts. Chapter II covers the kinetic studies designed to increase our understanding of the processes that create

and destroy BrNO molecules and Br atoms. Chapter III discusses the spectroscopic studies of the ro-vibrational spectra of BrNO. Each chapter includes a review of previous efforts, describes the apparatus and techniques used in these experiments, and discusses the results. A final chapter provides a summary of the overall effort and suggests future research.



## II. Kinetics

When bromine ( $\text{Br}_2$ ) and nitric oxide ( $\text{NO}$ ) are mixed in a darkened cell, chemical reactions take place that ultimately produce an equilibrium condition with static concentrations of  $\text{NO}$ ,  $\text{Br}_2$  and nitrosyl bromide ( $\text{BrNO}$ ). If the mixture is illuminated with a laser or other light source the  $\text{Br}_2$  and  $\text{BrNO}$  can be photodissociated, producing  $\text{Br}$  atoms and replenishing the  $\text{NO}$  concentration. (The strong  $\text{NO}$  bond is assumed to remain unbroken under the conditions considered in this research.) The chemical reactions determining the behavior of a mixture of  $\text{Br}_2$  and  $\text{NO}$  have been studied extensively, but little effort has gone into ensuring that the separate results obtained under a wide variety of experimental conditions provide a unified kinetic description. Recent efforts to describe the  $\text{Br}^*/\text{NO}$  laser (52) indicate that the results obtained so far do not accurately model the behavior of this system. Further study was therefore warranted.

The sections that follow detail the three phases of this investigation:

- In these experiments the concentrations of  $\text{NO}$ ,  $\text{Br}_2$  and  $\text{BrNO}$  when the light was applied were determined from the pressure decrease after the  $\text{NO}$  and  $\text{Br}_2$  were mixed. It was therefore necessary to reinvestigate the reaction of  $\text{NO}$  and  $\text{Br}_2$  in the absence of light to ensure that previously published results were correct and applicable to this experiment.
- After the light was applied the  $\text{Br}_2$  and  $\text{BrNO}$  concentrations were monitored by measuring the transmitted light intensity. The part of the absorption due to bromine was determined by applying the light to a cell containing only bromine while the part due to  $\text{BrNO}$  was found by driving the  $\text{Br}_2 + 2\text{NO} \rightleftharpoons 2\text{BrNO}$  reactions strongly towards  $\text{BrNO}$  using a large excess of  $\text{NO}$ . Comparing the results obtained during this phase with earlier efforts demonstrated that the apparatus used in these experiments provides trustworthy data.

- In the last phase the results of the initial investigations were combined to analyze the kinetics of a  $\text{Br}_2/\text{NO}/\text{BrNO}$  mixture exposed to light.

## 2.1 Previous Work

In 1968 Hisatsune and Zafonte (31) studied the reaction of  $\text{BrNO}$ ,  $\text{NO}$  and  $\text{Br}_2$  by mixing  $\text{NO}$  and  $\text{Br}_2$  and following the time dependence of the strong  $\text{NO}$  stretch infrared absorption band of the product  $\text{BrNO}$ . At about the same time, Ip and Burns (33) investigated the recombination of  $\text{Br}$  atoms in  $\text{He}$ ,  $\text{Ne}$ ,  $\text{Ar}$ ,  $\text{Kr}$ ,  $\text{N}_2$  and  $\text{O}_2$  from room temperature up to 1275 K following flash photolysis. A little later, in 1970, DeGraff and Lang (14) also studied the gas-phase recombination of  $\text{Br}$  atoms after flash photolysis of 2.2 to 3.3 torr of  $\text{Br}_2$  and found values for the rate constants that were in good agreement with the values previously obtained. Houel and van den Bergh (32) considered the equilibrium of  $\text{Br}_2$ ,  $\text{NO}$  and  $\text{BrNO}$  and determined the UV/Vis absorption spectrum of  $\text{BrNO}$ . In 1978 Hippler (30) once again studied the recombination of  $\text{Br}$  atoms after photolysis of less than 0.3 torr of  $\text{Br}_2$  at room temperature, this time in the range of 1-100 atm of the inert diluent  $\text{He}$ . They also studied the recombination of  $\text{Br}$  and  $\text{NO}$  in the presence of  $\text{He}$ . In 1979, Grimley and Houston (22) studied the primary and secondary photochemistry of  $\text{BrNO}$  by monitoring the infrared fluorescence from vibrationally excited  $\text{NO}$  following pulsed photolysis of  $\text{BrNO}$  at 355 nm and 490 to 650 nm. In 1986 Sedlacek and Wight (59) determined that Grimley and Houston were actually observing emission from  $\text{BrNO}$  excited by E-V energy transfer from excited  $\text{Br}$  atoms, not vibrationally excited  $\text{NO}$  molecules.

## 2.2 Safety Considerations

Bromine and nitric oxide are serious health hazards. Great care was taken throughout this experiment to avoid any direct exposure to these materials. Bromine, a dark red liquid at room temperature, volatilizes rapidly to form a red vapor with

a strong, disagreeable odor. The vapor is very irritating to the eyes and throat and the liquid causes painful sores when spilled on the skin (69). Nitric oxide is a colorless, poisonous gas that reacts rapidly with oxygen to form  $\text{NO}_2$ , a mildly poisonous brown vapor that is one of the principal components of smog.

### 2.3 Purification

The nitric oxide and bromine were purified prior to use. The NO (Matheson, 99% pure) was passed slowly through silica gel cooled to approximately  $-78^\circ\text{C}$  in a dry ice/acetone bath (Figure 2.1). A series of valves regulated the flow rate. After passing through the silica gel the NO was frozen in a tube cooled by liquid nitrogen ( $\text{LN}_2$ ). (NO melts at  $-163.6^\circ\text{C}$  and boils at  $-151.8^\circ\text{C}$ .) This allowed enough purified NO for several runs to be stored while maintaining a low reservoir pressure that would not prevent the flow of the NO over the silica gel. The NO was thawed as needed by removing the  $\text{LN}_2$  that surrounded the reservoir. The pressure was watched carefully and kept below 1 atm to minimize the risk that any NO would be vented into the laboratory; an NO-sensitive Spectra Physics gas detector monitored the area around the apparatus for leaks. Before each new batch of NO was purified the silica gel was warmed using heating tape to drive off the absorbed impurities.

The 99.5% pure bromine, from Spectrum Chemical Manufacturing, was cooled to  $-14^\circ\text{C}$  using a salt/ice mixture and the cell was evacuated to remove any impurities that do not freeze at this temperature. (Bromine melts at  $-7.2^\circ\text{C}$  and boils at  $58.78^\circ\text{C}$ .) The bromine was then further purified by repeated freeze/pump/thaw cycles. The bromine is frozen in a tube surrounded by liquid nitrogen, then a valve is opened and the tube evacuated so that any unfrozen impurities are removed. The liquid nitrogen is then removed and the pumping continued for a while to remove any frozen impurities that thaw before the bulk of the bromine. The valve to the pump is then closed and most of the remaining bromine cryogenically pumped to another tube. When a small amount of bromine remains in the original tube, the valve to

the second tube is closed and the first tube evacuated. This cycle is repeated several times. The purified bromine is allowed to thaw and kept in a reservoir until needed.

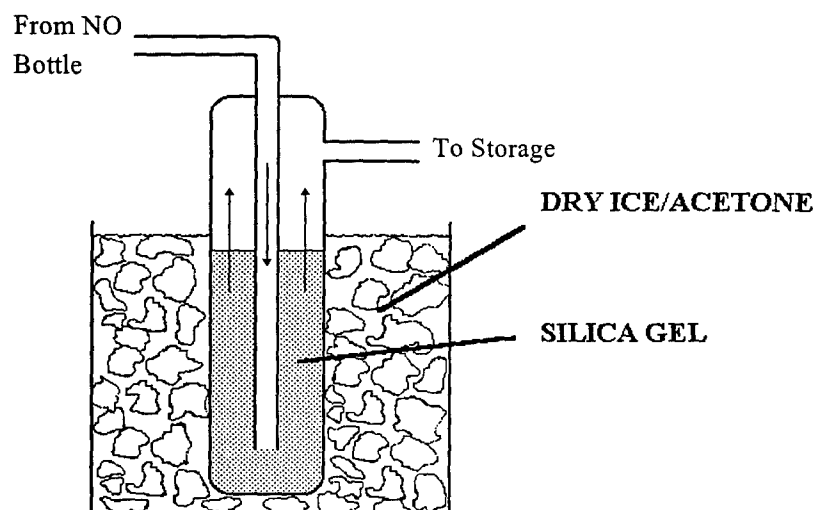


Figure 2.1 Apparatus used to purify NO.

#### 2.4 Apparatus

The apparatus used in this experiment is shown schematically in Figures 2.2 and 2.3. The Pyrex reaction cell, tubes, valves and other components were cleaned in acetone before assembly. The system was evacuated, checked for leaks, and then pumped on for several days to remove any residual acetone or other contaminants. A cold trap cooled by  $\text{LN}_2$  prevented any of the gases from contaminating the pump oil and improved the system vacuum. The mechanical pump proved capable of evacuating the apparatus to less than 0.01 torr. The cell pressure was measured using an MKS Instruments Model 690 Baratron 100 torr capacitance manometer with a heated head. The accuracy of this type of manometer is approximately 0.08% of the measured pressure, and the time constant of the gauge is  $< 25$  ms when the "fast" time constant is selected.

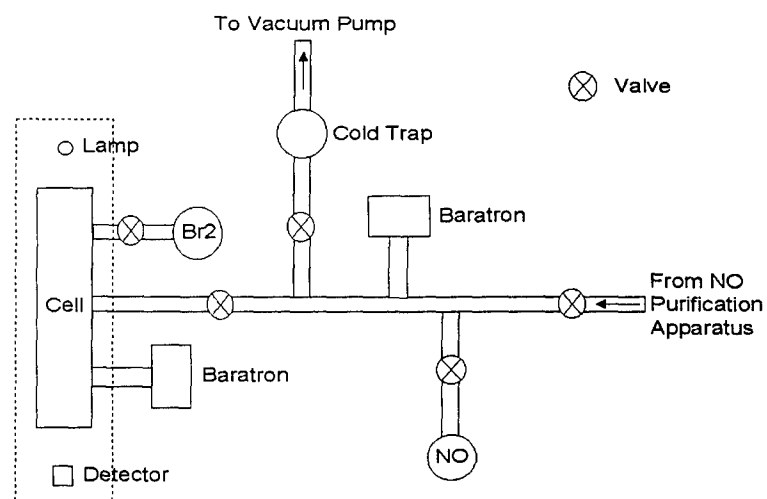


Figure 2.2 Schematic diagram of experimental apparatus.

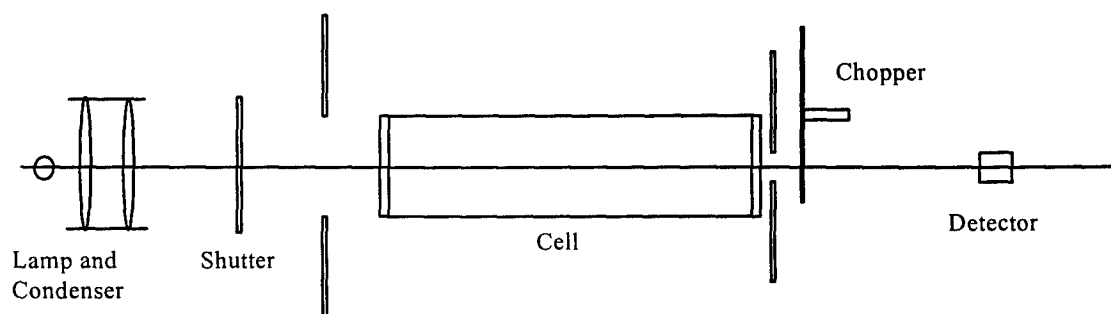


Figure 2.3 Reaction cell.

An Oriel high intensity halogen lamp with a 100W bulb (operated at 90W to prolong bulb life) provided the illumination. The lamp was powered by a stabilized DC power supply. The lamp and power supply were allowed to warm up for at least 30 minutes before any measurements were taken to increase the stability of the light output. Oriel (50) quotes less than .2 % change in lamp current and voltage over 8 hours after a 30 minute warm-up. A condenser using fused silica lenses collimated the beam before it entered the cell and the beam diameter was made slightly larger than the cell diameter to ensure that the cell was fully and evenly illuminated. The lamp and condenser give a useful spectral range of 240 to 2500 nm with high visible output (Figure 2.4) and the cell windows were made of  $\text{CaF}_2$  which is very transparent at these wavelengths (74). A cell with sealed Pyrex ends was also used in an effort to

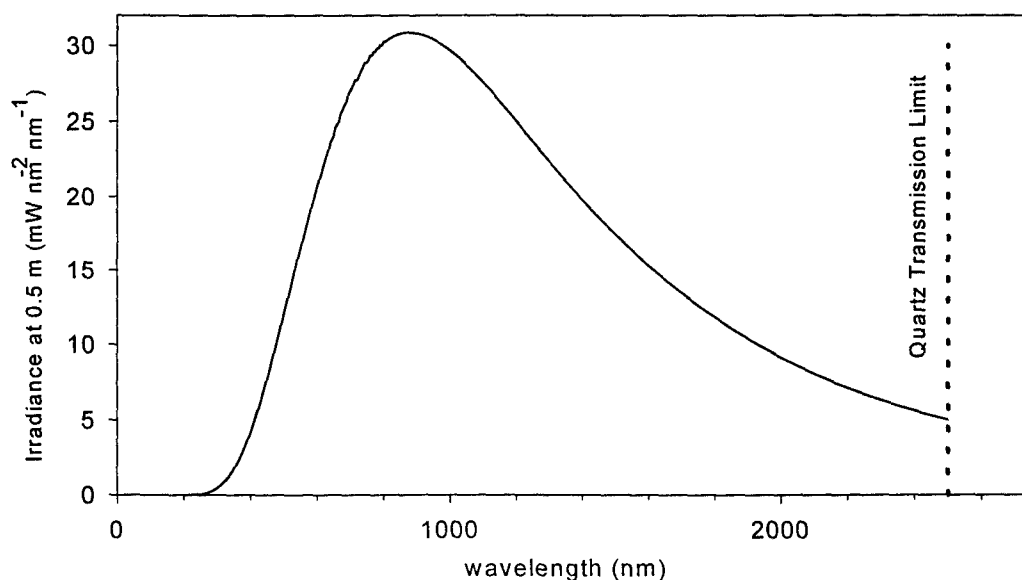


Figure 2.4 Oriel lamp output spectrum with quartz transmission cutoff. Curve represents blackbody emission for  $T = 3300\text{K}$ , the effective color temperature of the lamp (50).

eliminate  $\text{Br}_2$  absorption by the Torr-Seal used to attach the  $\text{CaF}_2$  windows. The light was chopped at 300 Hz, then passed through a 409 nm narrow-pass ( $10 \pm 2$

nm) filter (chosen to match the maximum in the bromine absorption curve) and detected by a Hamamatsu photodiode. Another photodiode monitored the lamp directly to detect changes in the incident light intensity; additionally, the transmitted light intensity through an empty cell was checked routinely. The signals from the photodiodes and the cell manometer were sent to a Stanford Research Systems lock-in amplifier to be digitized and recorded. The light intensity was assumed to be proportional to the detector output voltage and only relative light intensities were determined.

A Melles Griot manually-activated shutter (model 04-IMS-005) controlled cell illumination. The specifications on the shutter indicate that it opens fully in less than a sixtieth of a second ( $\frac{1}{60}$ ). Detector output with an empty cell reached a steady value less than .04 seconds after the shutter was opened or closed (Figure 2.5).

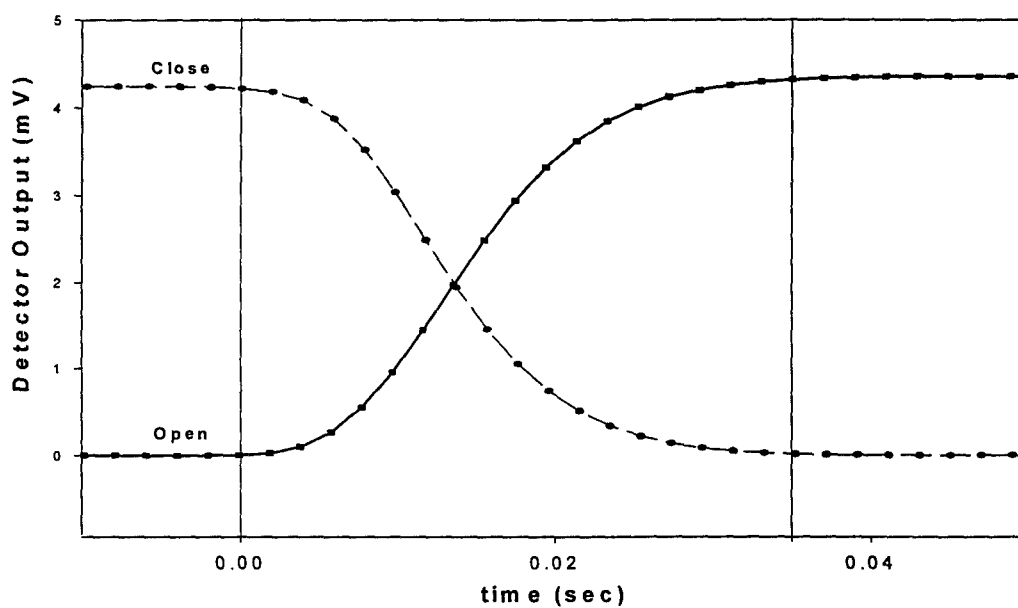


Figure 2.5 Detector output when the shutter is opened and closed, using empty cell. Recorded at 512 Hz digitization rate.

The effect of varying the light intensity was investigated using neutral density filters placed between the lamp and the cell. The bandpass filter in front of the

detector ensures that the detector sees only a narrow portion of the incident light spectrum. The detector output is an accurate indication of the integrated intensity only if the overall shape of the spectrum of the incident light does not change. Changing the intensity by reducing the lamp voltage would change the temperature of the filament and thereby alter the spectrum of the incident light, but if the intensity is reduced using neutral density filters with flat absorption curves over the wavelengths of interest the overall shape of the spectrum is not changed.

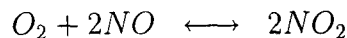
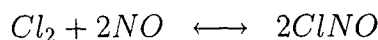
No provision was made to control the temperature of the cell but the temperature at the exterior surface of the cell was monitored with a thermocouple and only runs made when this temperature was  $293 \pm 1$  K were used in the analysis. The cell was kept covered to prevent any possible complications due to room light.

## 2.5 Dark Reactions

**2.5.1 Mechanism.** When  $\text{Br}_2$  and NO are mixed in a cell, the two gases react to form BrNO while a back reaction regenerates  $\text{Br}_2$  and NO:



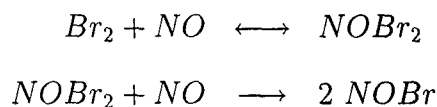
The  $\text{Br}_2 + 2\text{NO}$  reaction is third-order. Third-order bond-breaking reactions between stable molecules are quite rare and all known examples involve nitric oxide as one of the reactants (42). The two best-understood reactions are those involving chlorine and oxygen:



The collision of three molecules is so unlikely that chemists prefer to picture the reaction as consisting of two steps. One proposed mechanism for the reaction with



bromine is



In this scheme a small concentration of  $\text{NOBr}_2$  is maintained in equilibrium with  $\text{NO}$ ,  $\text{Br}_2$  and  $\text{NOBr}$ . Another postulated mechanism predicts a small equilibrium concentration of  $\text{NO}$  dimers, but in general the identity of the intermediate product does not matter as long it is in equilibrium with the reacting molecules. No experiment, however, has ever provided convincing evidence for the existence of any intermediate complex (31).

Considering only the forward and reverse reactions of Equation 2.1, the rate of change of the concentration of each species is

$$\frac{d[\text{Br}_2]}{dt} = -k_f[\text{Br}_2][\text{NO}]^2 + k_r[\text{BrNO}]^2 \quad (2.2)$$

$$\frac{d[\text{NO}]}{dt} = -2k_f[\text{Br}_2][\text{NO}]^2 + 2k_r[\text{BrNO}]^2 \quad (2.3)$$

$$\frac{d[\text{BrNO}]}{dt} = -\frac{d[\text{NO}]}{dt} \quad (2.4)$$

Equation 2.4 holds as long as the N-O bond is not broken and all the  $\text{NO}$  is present either as  $\text{NO}$  or in  $\text{BrNO}$  molecules.

The standard SI unit of concentration is moles per cubic decimeter ( $\text{mol/dm}^3$ ), but multiplying by Avogadro's Number and converting to centimeters gives molecules per cubic centimeter ( $\text{molecules/cm}^3$ ), which is more convenient for gas phase reactions (61). The equation of state for an ideal gas relates the concentration (number density)  $[M] = n/V$  in these units to the pressure and temperature of the gas:

$$\begin{aligned} P &= \left(\frac{n}{V}\right) k_B T \\ P(M) &= 1.035579 \times 10^{-19} [M] T \end{aligned} \quad (2.5)$$

with the pressure in torr and temperature in Kelvins. Since the manometer measures total pressure, not concentration, Equation 2.5 must be used to relate the concentration changes given by the solution of Equations 2.2-2.4 to the change in the cell pressure. In these experiments it is assumed that the total pressure is the sum of the partial pressures which are related to the concentrations by Equation 2.5 with, unless otherwise noted,  $T = 293 \pm 1$  K.

The molecular concentrations, rewritten in terms of a progress variable  $x(t)$ , are

$$[Br_2](t) = [Br_2]_0 - x(t) \quad (2.6)$$

$$[NO](t) = [NO]_0 - 2x(t) \quad (2.7)$$

$$[BrNO](t) = [BrNO]_0 + 2x(t) \quad (2.8)$$

and the total cell pressure is

$$P^T = P_0^T - P(x(t)) \quad (2.9)$$

where  $P(x(t)) = x(t) k_B T$  is the pressure equivalent to the concentration  $[x(t)]$ . The differential equation for  $x(t)$  is

$$\frac{dx}{dt} = k_f([Br_2]_0 - x)([NO]_0 - 2x)^2 - k_r([BrNO]_0 + 2x)^2 \quad (2.10)$$

which gives

$$\int_{t_0}^t dt = \frac{1}{k_f} \int_0^x \frac{dx}{([Br_2]_0 - x)([NO]_0 - 2x)^2 - K_{eq}^{-1}([BrNO]_0 + 2x)^2} \quad (2.11)$$

where

$$K_{eq} = \frac{k_f}{k_r} \quad (2.12)$$

Integrating the  $x$ -dependent part of Equation 2.11 requires that the roots of the cubic polynomial in the denominator be determined. The integrand is then expressed in terms of partial fractions and integrated to give  $f(x, [BrNO]_0, [Br_2]_0, [NO]_0, K_{eq})$ . The result can be solved to give  $x$  as an analytic function of time, but it is more convenient to invert the  $x(t)$  data obtained after NO and Br<sub>2</sub> are mixed and fit the resulting  $t(x)$  data to  $f(x, [BrNO]_0, [Br_2]_0, [NO]_0, K_{eq})$  by varying  $k_f$ :

$$t(x) - t_0 = \frac{1}{k_f} f(x, [BrNO]_0, [Br_2]_0, [NO]_0, K_{eq}) \quad (2.13)$$

From  $k_f$  and  $K_{eq}$  the value of  $k_r$  is determined. Since  $k_f$  simply scales the integrated equation the fit consists of varying  $k_f$  until the model curve overlays the data. This simplicity is lost if one or more additional quantities, such as  $K_{eq}$  or  $[NO]_0$ , are also taken as fit parameters, but using Mathematica to integrate Equation 2.11 allows the effect of varying these quantities to be easily determined. In any case, the model curve can be fit to the data with a least squares procedure, using Tablecurve or a similar software package, to determine the values of the parameters and their uncertainties.

Figure 2.6 is a plot of the total pressure versus time when 39.67 torr of NO was added to 9.38 torr of Br<sub>2</sub>. As the forward and back reactions in equation 2.1 approach equilibrium,  $x(t)$  and the concentrations approach their final values. If  $x_f$  is  $x(t \rightarrow \infty)$  the rate of change of  $x$  (Equation 2.10) can be set equal to zero to obtain the value of  $K_{eq}$ :

$$K_{eq} = \frac{([BrNO]_0 + 2x_f)^2}{([Br_2]_0 - x_f)([NO]_0 - 2x_f)^2} \quad (2.14)$$

Previous measurements of the forward reaction rate have generally been obtained using pseudo-first order (excess NO) or pseudo-second order (excess Br<sub>2</sub>) techniques that ignore the reverse reaction. The equilibrium constant has been de-

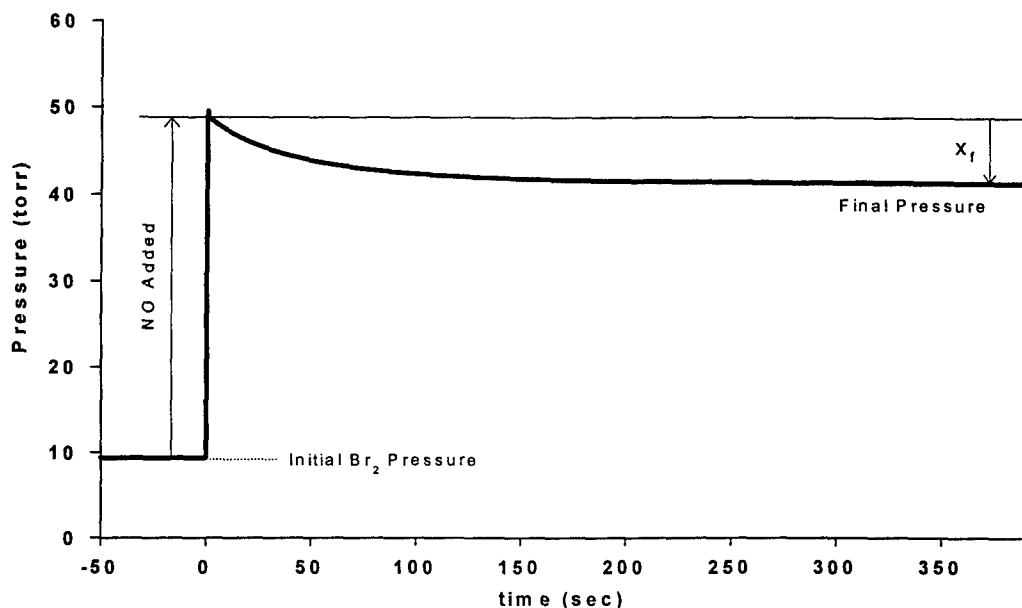


Figure 2.6 Pressure vs. time after 39.67 torr of NO was added to 9.38 torr of Br<sub>2</sub>.

terminated by measuring the final pressure after known quantities of Br<sub>2</sub> and NO are mixed. The technique described above connects these two techniques by characterizing the entire reaction from initial mixing to steady state.

**2.5.2 Experimental Procedure.** Br<sub>2</sub> was flowed into the cell and its pressure monitored. Once the Br<sub>2</sub> pressure reached its desired value (typically 5 to 10 torr) the valve on the Br<sub>2</sub> reservoir was closed. The valve between the NO reservoir and an intermediate reservoir was then opened and the frozen NO in the reservoir thawed until the desired initial pressure of NO (less than 1 atm) was reached. The NO reservoir was then closed and the liquid nitrogen reapplied. The valve between the intermediate NO reservoir and the cell was opened quickly to allow some of the NO to mix with the Br<sub>2</sub>, then closed almost immediately so that the NO reservoir pressure remained significantly higher than the pressure in the cell. The high NO pressure in the intermediate reservoir ensured that the NO flowed rapidly into the cell and that little Br<sub>2</sub> left the cell as the NO entered. The total pressure in the cell

after the NO was added was held to less than 100 torr so that the range of the 100 torr manometer was not exceeded. A 1000 torr manometer head would have allowed higher total pressures but the pressure in the intermediate NO reservoir would then have dropped too far to ensure that little bromine escaped when the NO was added. With practice the amount of NO allowed to enter the cell could be controlled to within about 5 torr by varying the time that the valve was open. The cell pressure was monitored until steady-state conditions were established.

When the NO was injected into the cell the pressure measurement displayed a transient high reading due to the response of the manometer to the high pressure wave of entering gas. Figure 2.7 shows this effect when NO is added to NO and argon is added to bromine. In both cases no chemical reactions occur and the pressure levels out in about 2 seconds. The reaction that occurs when NO is added to Br<sub>2</sub> causes

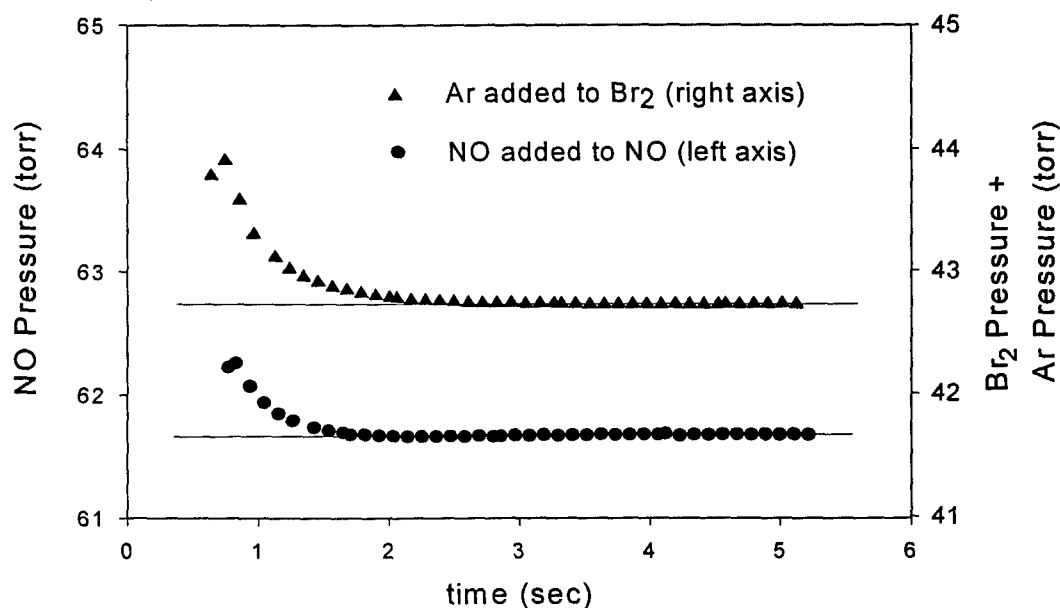


Figure 2.7 Examples of rapidly-damped pressure transient when NO is added to NO and Ar is added to Br<sub>2</sub>.

the pressure to drop instead of leveling out. The pressure drop immediately after the NO is added is almost linear and the beginning NO pressure may be determined

by extrapolating the pressure to  $t = 0$ . This determination of initial NO pressure ignores any effects from the finite time required to mix the gases. In the example shown in Figure 2.8 the maximum pressure is reached less than .6 seconds after the cell pressure begins to rise and the transient disappears a little over a second later.

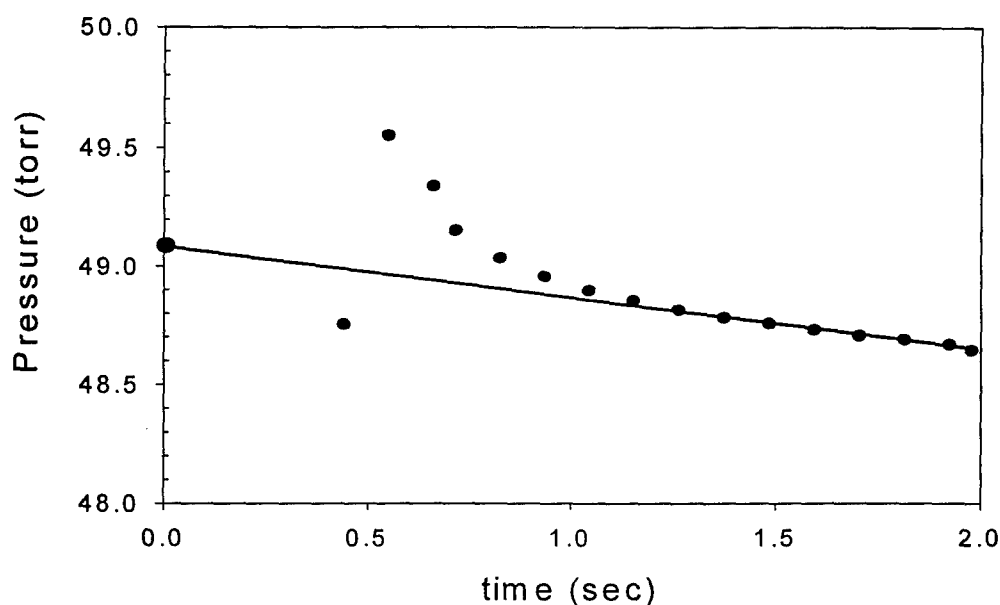


Figure 2.8 Example of pressure transient when NO is added to Br<sub>2</sub>.

**2.5.3 Results.** Figure 2.9 is a representative example of the results obtained when Equation 2.13 is used to model the  $t(x)$  data. This case corresponds to the pressure vs. time data shown in Figure 2.6, with  $P_0(\text{Br}_2) = 9.38$  torr,  $P_0(\text{NO}) = 39.67$  torr and  $K_{\text{eq}} = .214$  torr<sup>-1</sup>. The value of  $k_f$  determined from the fit is  $1.5247 \pm .0004 \times 10^{-5}$  torr<sup>-2</sup> s<sup>-1</sup> at 293K, or  $1.2186 \pm .3197 \times 10^{-38}$  cm<sup>6</sup>/molecule<sup>2</sup>-s. The inset view for small  $x$  and  $t$  shows that the initial pressure drop is very linear, so extrapolating the initial pressure to  $t = 0$  provides a reliable determination of the

starting NO pressure. Equation 2.13 evaluated for this case, with  $P(x)$  in torr, is

$$\begin{aligned} k_f t(P(x)) = & -0.001823 - 0.000841 \arctan[0.0411509 (2 P(x) - 36.80)](2.15) \\ & + 0.00047 \ln[P(x)^2 - 36.80 P(x) + 486.212] \\ & - 0.000945 \ln(7.59 - P(x)) \end{aligned}$$

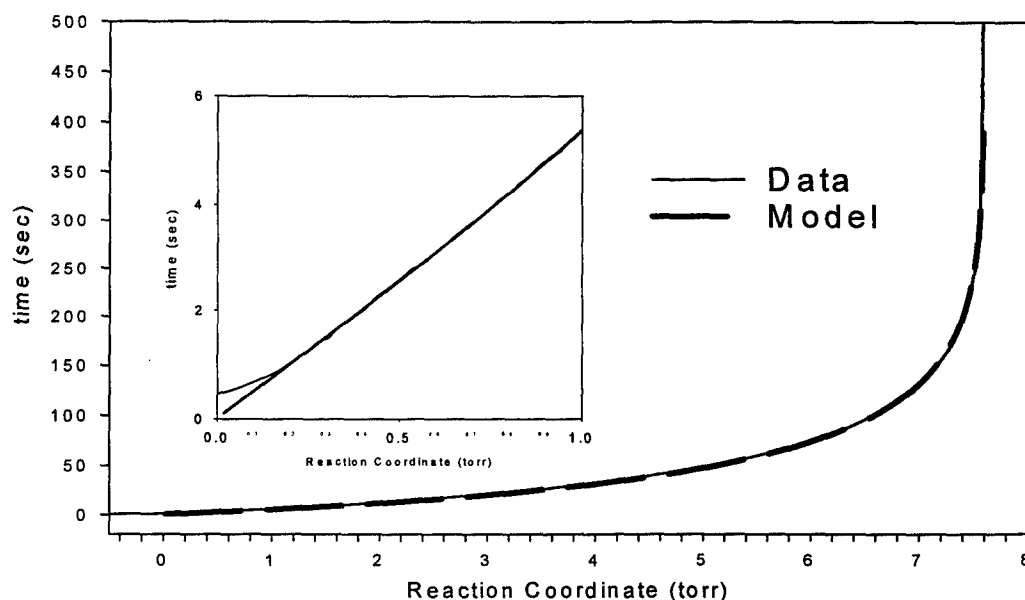


Figure 2.9 The dark reaction model fit to the data of Figure 2.6.

The values of the rate constants and the equilibrium constant determined in this experiment are listed in Table 2.1 along with results from previous efforts. The data used to determine  $K_{eq}$  and  $k_f$  are shown in Tables 2.2 and 2.3 and the range of initial  $Br_2$  and NO pressures is shown in Figure 2.10. As explained in the next section, the data in the second table could not be used to calculate  $K_{eq}$  but was used to find  $k_f$ . The rate constant for the reverse reaction, calculated using the experimental values of  $K_{eq}$  ( $6.71 \pm .92 \times 10^{-18} \text{ cm}^3/\text{molecule}$ ) and  $k_f$  ( $1.40 \pm .18 \times 10^{-38} \text{ cm}^6/\text{molecule}^2\text{-s}$ ), is  $2.09 \pm .55 \times 10^{-21} \text{ cm}^3/\text{molecule-s}$  at 293K.

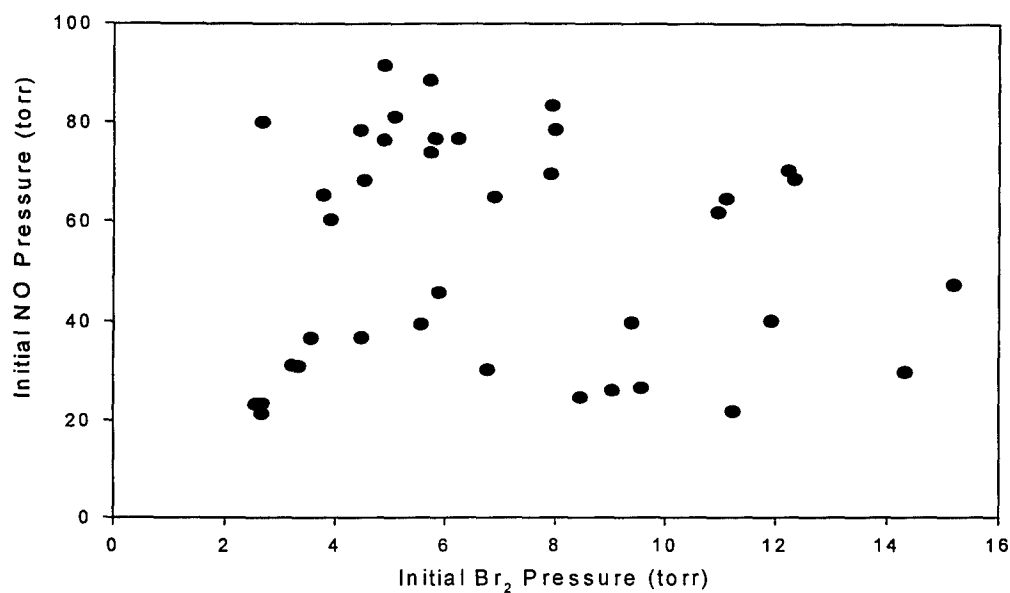


Figure 2.10 Range of initial Br<sub>2</sub> and bromine pressures used in determination of  $K_{eq}$  and  $k_f$ .

Table 2.1 Values of  $K_{eq}$ ,  $k_f$  and  $k_r$  obtained in this and previous efforts. The quantities listed for this study are the means  $\pm 1\sigma$  determined from the data in Tables 2.2 and 2.3.

	This Effort	Hisatsune (31)	Hippler (30)	Houel (32)
$K_{eq}$ ( $\text{atm}^{-1}$ )	$168 \pm 23$	89		$150 \pm 48$
$k_f$ ( $10^{-38} \text{ cm}^6/\text{molecules}^2\text{-s}$ )	$1.40 \pm .18$	$1.32 \pm .14$	$1.68 \pm 0.11$	$1.60 \pm 0.16$
T (K)	$293 \pm 1$	303	298	$303 \pm 0.5$



Table 2.2 Data used to determine rate constants.

$P_0(\text{Br}_2)$ (torr)	$P_0(\text{NO})$ (torr)	$P(x_f)$ (torr)	$K_{eq}$ ( $\text{atm}^{-1}$ )	$k_f$ ( $10^{-38} \text{ cm}^6/\text{molecule}^2\text{-s}$ )
11.24	21.81	5.46	132.2	1.040
14.33	29.84	7.63	124.3	1.236
9.56	26.63	6.06	151.5	1.051
9.03	26.1	5.95	173.3	1.210
8.45	24.66	5.55	175.6	1.301
15.20	47.38	11.20	152.8	1.208
11.92	40.05	9.25	209.8	1.222
9.38	39.67	7.59	162.4	1.219
6.78	30.31	5.38	164.5	1.289
12.34	68.44	11.14	147.5	1.252
10.96	61.74	9.86	152.2	1.531
12.23	70.24	11.33	191.5	1.490
11.11	64.47	10.21	181.5	1.088
5.56	39.45	5.06	181.0	1.344
5.89	45.77	5.49	189.2	1.295
2.67	21.38	2.29	148.7	0.901
4.48	36.79	4.13	182.0	1.210
2.67	23.36	2.33	138.8	0.999
7.91	69.47	7.45	123.2	1.288
2.56	23.33	2.34	217.5	1.038
3.34	31.03	3.07	171.3	1.128
6.90	64.8	6.61	172.1	1.115
3.23	31.21	3.02	208.4	1.611
7.99	78.43	7.71	162.6	1.368
3.56	36.66	3.34	171.5	1.014
7.94	83.33	7.69	155.7	1.074
6.23	76.59	6.09	194.1	0.923
5.74	73.81	5.59	161.4	1.574
5.81	76.59	5.67	163.9	1.120
4.52	68.2	4.41	152.5	1.280
3.91	60.26	3.81	159.2	1.065
5.72	88.4	5.62	161.3	1.165
4.88	76.34	4.79	173.9	1.295
5.08	81.03	5.00	188.3	1.232

Table 2.3 Data used to determine  $k_f$  only.

$P_0(\text{Br}_2)$ (torr)	$P_0(\text{NO})$ (torr)	$P(x_f)$ (torr)	$k_f$ ( $10^{-38}$ cm <sup>6</sup> /molecule <sup>2</sup> -s)
4.52	68.2	4.57	1.339
3.91	60.26	3.95	1.254
5.72	88.4	5.89	1.168
4.88	76.34	4.89	1.216
5.08	81.03	5.13	1.230
3.78	65.25	3.90	1.235
4.45	78.34	4.54	1.161
4.89	91.41	5.04	1.253
2.67	79.99	2.84	1.216

*2.5.4 Error Sources.* The error in the forward rate is caused by uncertainties in the pressure measurements and temperature variations between runs. The initial bromine pressure and the cell pressure after the NO is added are in error by no more than  $\pm .01$  torr. The error in the initial NO pressure, however, is larger because that pressure is determined by extrapolating the initial linear pressure decrease. The estimated error in the initial NO pressure is .02 torr.

Temperature variations also change the pressure in the cell. The temperature inside the cell was not monitored but the relatively low heat capacity of the gas ensures that it is in thermal equilibrium with the cell. The heat capacity of the cell prevents sudden temperature variations and the room temperature never changed by more than  $\pm .2$  C over the course of a run. A temperature change this large at 293K changes the pressure of 50 torr of an ideal gas by  $\pm .034$  torr.

The uncertainty in the reverse rate, 27%, is twice that of the forward rate because of the uncertainty in the equilibrium constant:

$$\begin{aligned}
 \Delta k_r &= \Delta k_f \frac{1}{K_{eq}} + \Delta K_{eq} \frac{k_f}{(K_{eq})^2} \\
 &= (.16 \times 10^{-38}) \frac{1}{6.23 \times 10^{-18}} + (.84 \times 10^{-18}) \frac{1.21 \times 10^{-38}}{(6.23 \times 10^{-18})^2} \\
 &= 2.57 \times 10^{-22} + 2.62 \times 10^{-22} \text{ cm}^3/\text{molecule} - \text{s}
 \end{aligned}$$

The value of the equilibrium constant determined using Equation 2.14 depends on  $x_f$  which in turn depends on the final, steady-state cell pressure. Figure 2.11 shows the variation in  $K_{eq}$  for a  $\pm .1$  torr error in the final pressure, with  $[Br_2]_0 = 5$  torr and  $[NO]_0 = 5 - 70$  torr. The effect is larger when the initial NO pressure is high and the final pressure is too low; when  $[NO]_0 = 70$  an error of  $-.05$  torr ( $-0.07\%$  of the nominal final pressure of  $70.12$  torr) makes the calculated equilibrium constant  $.37 \text{ torr}^{-1} \text{ s}^{-1}$  versus the nominal value of  $.221 \text{ torr}^{-1} \text{ s}^{-1}$ . The resulting value for the reverse reaction rate is  $.60$  times its nominal value. Under these conditions the bromine concentration in steady state is very low and small changes in the final pressure have a large influence on  $K_{eq}$  through the  $[Br_2]_0 - x_f$  term in the denominator of Equation 2.14.

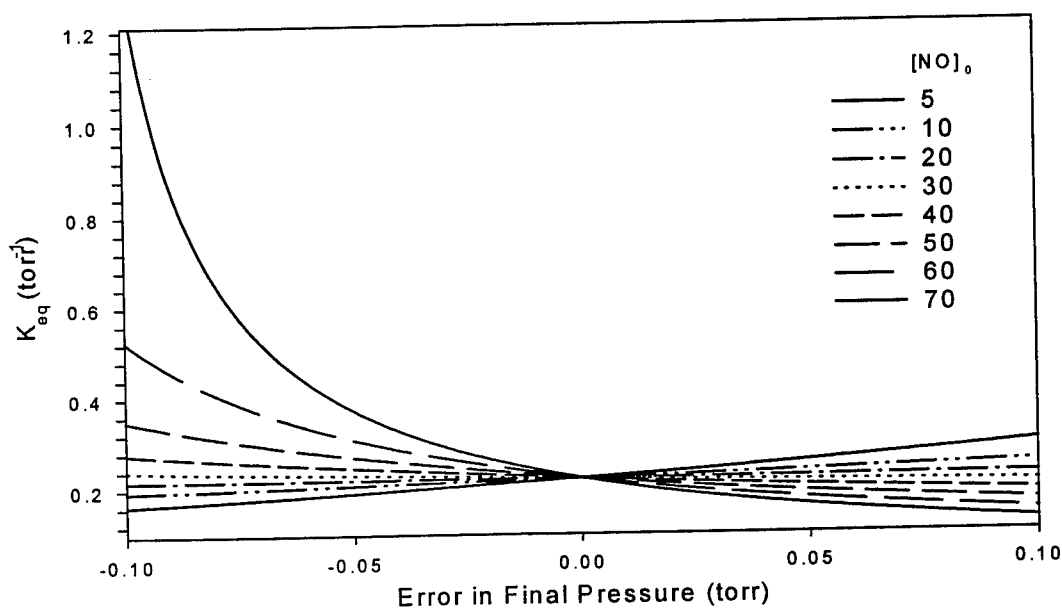


Figure 2.11 Calculated value of the equilibrium constant vs. error in final pressure for an initial  $Br_2$  pressure of 5 torr and a range of initial NO pressures. The nominal value of the equilibrium constant is  $.221 \text{ torr}^{-1}$ .

Errors in the determination of the final pressure affect the value of  $x_f$  but other error sources are also present. The error in the initial NO pressure directly

affects the calculated value of  $x_f$ . In addition to changing the pressure directly, temperature variations alter the final pressure indirectly by changing the equilibrium constant. The consequent change in the steady-state pressure, calculated using the reported value (32) of  $-10.71 \pm 1.86$  kcal/mol for  $\Delta H^0$ , is shown in Figure 2.12. (See Section 2.7.6.) For the pressures used in this experiment a temperature change of  $\pm 1$  K changes the pressure by no more than 0.05 torr. Both temperature effects push the final pressure up when the temperature increases.

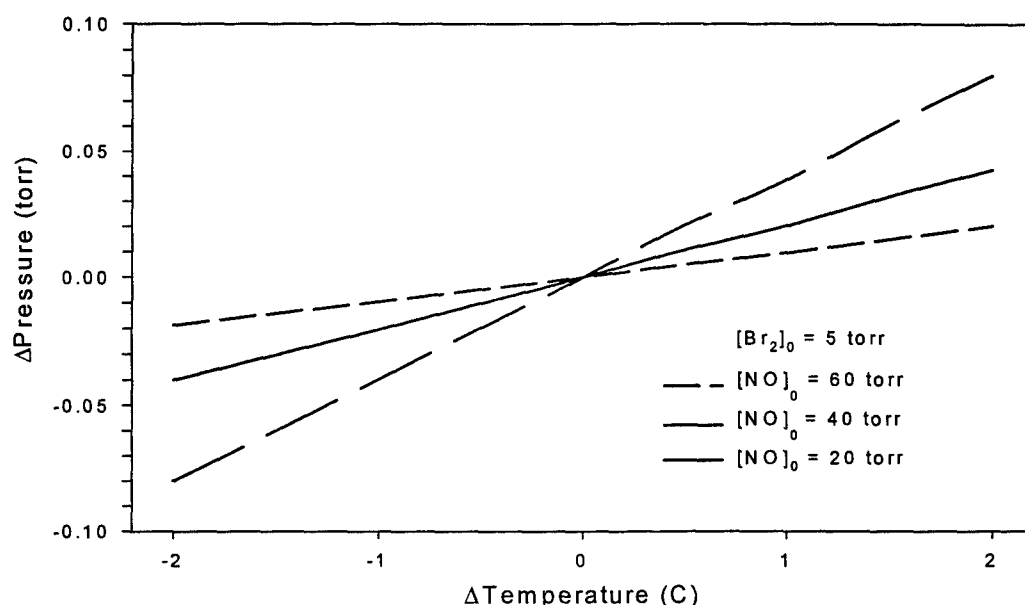


Figure 2.12 Calculated change in steady-state pressure caused by temperature dependence of the equilibrium constant, using  $\Delta H^0 = -10.71 \pm 1.86$  kcal/mol, for  $K_{eq}$  equal to  $.221 \text{ torr}^{-1}$  at 293K.

Another effect that reduces the final pressure is bromine adsorption onto the internal surfaces of various parts of the apparatus after the NO is added. The components in contact with the bromine included the glass cell, the  $\text{CaF}_2$  windows, the Torr-Seal used to attach the windows, a short piece of stainless steel tubing used to connect the cell to the manometer, the manometer itself, and the O-rings on the valves. The bromine loss, most obvious after the components of the apparatus were

cleaned, is difficult to quantify because the loss rate depends on the history of the cell and cannot be measured independently of the change in total pressure after the NO is added. The pressure of an NO sample in a clean cell showed no tendency to decrease and when a large excess of NO was added to bromine to drive the bromine concentration almost to zero the pressure also remained steady, indicating that BrNO is not easily absorbed.

No fully satisfactory solution to the bromine absorption problem was found. Eliminating the Torr-Seal by using a cell with sealed Pyrex ends reduced the problem somewhat. Since the manometer is an essential part of the experiment it could not be removed but the metal tube connecting the manometer to the cell was made as short as possible. The cell, tube and manometer were "seasoned" after adding bromine by allowing the pressure to drop until it reached a steady value before adding the NO. Although this technique allows the cell pressure to stabilize when only Br<sub>2</sub> is present (35), after Br<sub>2</sub> is removed by reaction with NO the balance between the bromine atoms absorbed onto the walls and those in the gas phase is disturbed and more bromine may become available to react. Additionally, if a cell that has had bromine in it is evacuated, then filled with NO, the transmitted light intensity gradually drops, indicating that the NO (which does not absorb light at these wavelengths) is pulling bromine off the cell walls or other components to form BrNO. (Since the number of molecules in the gas phase does not change, the cell pressure is not affected.)

The loss of Br<sub>2</sub> to the walls explains the long-term pressure decrease sometimes seen after the NO, Br<sub>2</sub> and BrNO pressures should have equilibrated. The long-term pressure drop was usually very linear so a correction proportional to time suggested itself. Figure 2.13 shows a pressure trace before and after the application of a linear correction. In this example 13.5 torr of Br<sub>2</sub> and 62.0 torr of NO were mixed. If the equilibrium constants determined in this and other experiments are correct the pressure should drop by no more than .016 torr after  $t = 180$  seconds

but the observed pressure drops .06 torr from  $t = 180$  to  $t = 220$  seconds and is still dropping approximately linearly. Forcing the pressure to level out after enough time had passed to ensure that the continuing decline was not the result of the chemical reactions changed the overall shape of the pressure curve very little and gave rate constants in good agreement with those obtained when no correction was needed.

In the runs listed in Table 2.3 an excess of NO was added to the bromine. The cell pressure dropped rapidly, reaching equilibrium in a few minutes but at a final pressure indicating that more bromine had reacted than was originally present. The equilibrium constant calculated from the final pressure is then infinite but the value of  $k_f$  may still be determined by assuming that the equilibrium constant has the value determined from the rest of the runs and fitting the data as before. The resulting value of  $k_f$  is insensitive to the value of  $K_{eq}$  chosen.

In Figure 2.14  $K_{eq}$  and  $k_f$  for each run is plotted as a function of the ratio of the initial NO pressure to the initial bromine pressure. With the corrections to  $x_f$  neither the equilibrium constant nor the forward rate constant exhibit a statistically significant dependence on the ratio.

*2.5.5 Summary.* The agreement between the data and the model demonstrated by the new fitting technique provides further evidence that the reaction of  $\text{Br}_2$  and NO is adequately described by third-order kinetics. The values of the rate constants are consistent with those determined previously.

The papers reporting the results of previous efforts to determine the forward rate constant and the equilibrium constant for the  $\text{Br}_2 + 2 \text{NO} \rightleftharpoons 2 \text{BrNO}$  reactions do not mention the absorption of bromine by the walls or other parts of the apparatus. It is therefore difficult to determine if this problem influenced any of the earlier results. It is clear from this study that loss of bromine to the walls of the apparatus can introduce significant errors into the determination of the rates.

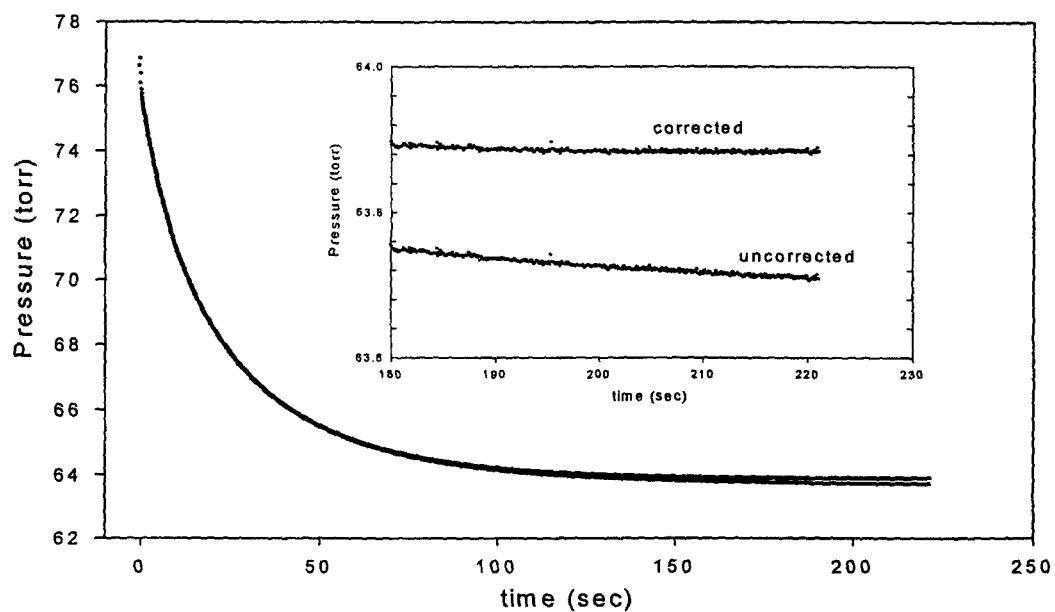


Figure 2.13 Example of long-term pressure decline after 13.5 torr  $\text{Br}_2$  and 62.0 torr NO were mixed, and same data with linear correction.

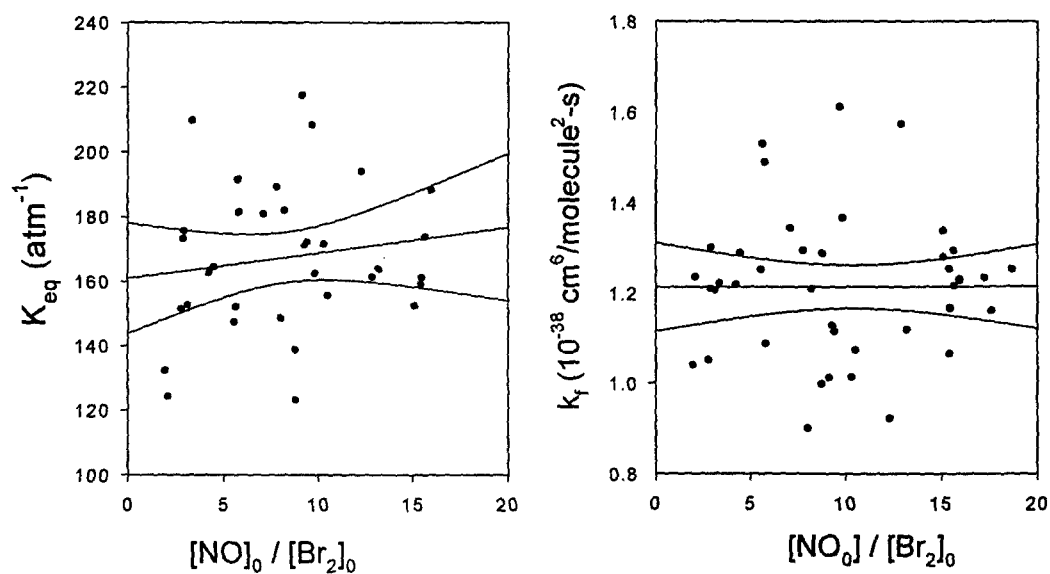


Figure 2.14  $K_{\text{eq}}$  and  $k_f$  vs. ratio of initial NO and  $\text{Br}_2$  pressures, with linear least squares fits and 95% confidence intervals.

## 2.6 Bromine Dissociation and Absorption Cross Section

As discussed in Chapter III, molecules absorb and emit light at discrete wavelengths as they jump between quantized energy levels. Molecules may also absorb across a continuous range of wavelengths, but in this case at least one of the states must be dissociative (8). If the light absorbed by a molecule is sufficiently energetic the bonds holding the atoms together will be severed; a diatomic molecule like  $\text{Br}_2$  will be split into two atoms. The most common type of photodissociation for triatomic molecules is (49)



where the X-Y bond is weaker than the Y-Z bond. Photodissociation therefore occurs by absorption of light with energies exceeding that required to break the weakest bond in the molecule, although less energetic photons may dissociate a molecule already in a high vibrational or rotational state. Any energy in excess of that required to sever the bond is distributed among the dissociation fragments, increasing their kinetic energy or raising them to excited rotational or vibrational states.

*2.6.1 Photodissociation of Bromine.* This section describes the determination of the molecular bromine absorption cross section. Additionally, the photodissociation of bromine is analyzed to aid the later analysis of the behavior of an illuminated mixture of  $\text{Br}_2$ , NO and  $\text{BrNO}$ .

With the apparatus used in this experiment there is a small pressure rise when a cell filled only with  $\text{Br}_2$  is illuminated (Figure 2.15). The pressure increases because the photodissociation of a fraction of the bromine atoms increases the number of particles in the cell. Since each dissociated bromine molecule produces two bromine atoms the molecular bromine and bromine atom concentrations after illumination



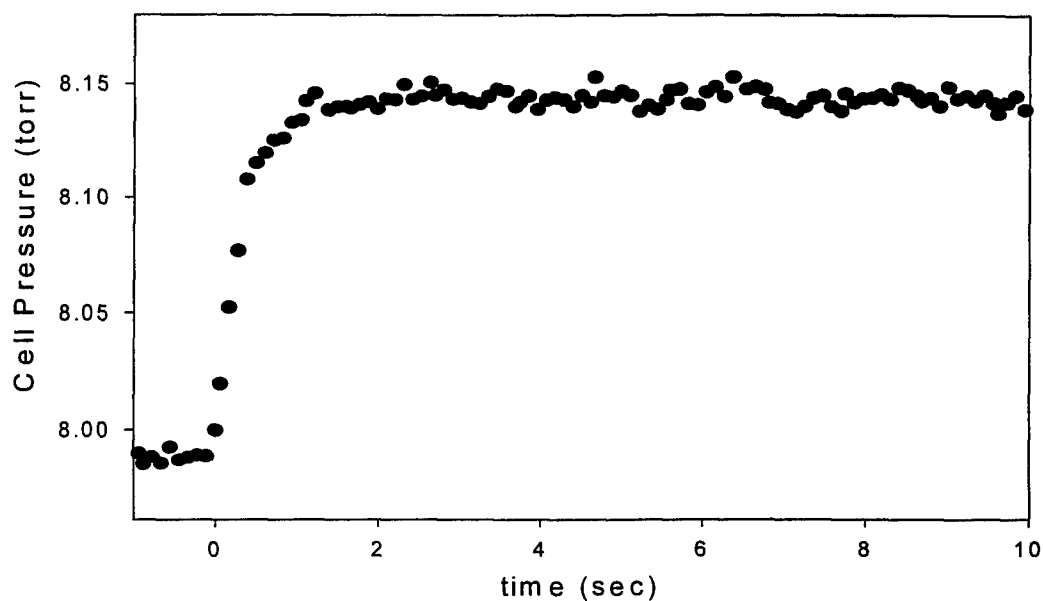


Figure 2.15 Cell pressure measured by manometer when 7.9 torr of  $\text{Br}_2$  is illuminated.

are related to  $[\text{Br}_2]_0$ , the bromine concentration before the light is turned on, by

$$[\text{Br}_2]_0 = \frac{1}{2}[\text{Br}] + [\text{Br}_2] \quad (2.17)$$

The total pressure is then

$$P^T = 2P(\text{Br}_2)_0 - P(\text{Br}_2) \quad (2.18)$$

and the change in the total pressure after the light is turned on is

$$\begin{aligned} \Delta P^T &= P(\text{Br}) + P(\text{Br}_2) - P(\text{Br}_2)_0 \\ &= \frac{1}{2}P(\text{Br}) \end{aligned} \quad (2.19)$$

In addition to the pressure change after the shutter is opened, the transmitted light intensity also varies. The transmitted light intensity provides a direct mea-

surement of the concentration of bromine molecules because bromine atoms do not absorb light at the wavelengths used in this experiment. If the gas temperature increases the pressure will rise linearly with the absolute temperature but as long as the cross section for absorption is independent of temperature the transmitted intensity will change only if the processes that counter bromine dissociation are temperature dependent. Monitoring the light intensity therefore allows at least part of any temperature effects to be discerned from concentration changes.

*2.6.2 Bromine Absorption Cross Section.* By the Beer-Lambert Law the intensity of a parallel beam of monochromatic light after passing through a length  $l$  of gas is

$$I = I_0 e^{-(\sigma c l)}$$

or

$$I = I_0 10^{-(\epsilon N l)} \quad (2.20)$$

where  $I_0$  is the intensity detected when the cell is empty,  $c$  is the concentration in moles/liter,  $N$  is the number of molecules per  $\text{cm}^3$ , and  $l$  is in centimeters (49). The absorption coefficient  $\epsilon$  (liter/mole-cm) is related to the absorption cross section  $\sigma$  ( $\text{cm}^2$ ) by

$$\sigma = \frac{\epsilon \ln(10) 10^3}{6.022 \times 10^{23}}$$

Figure 2.16 depicts the  $\text{Br}_2$  absorption coefficient for wavelengths from 200 to 600 nm and also shows the output of the Oriel lamp at these wavelengths.

Solving Equation 2.20 for the  $\text{Br}_2$  concentration gives

$$[\text{Br}_2] = -\frac{1}{\sigma_{\text{Br}_2} l} \ln \left( \frac{I}{I_0} \right) \quad (2.21)$$

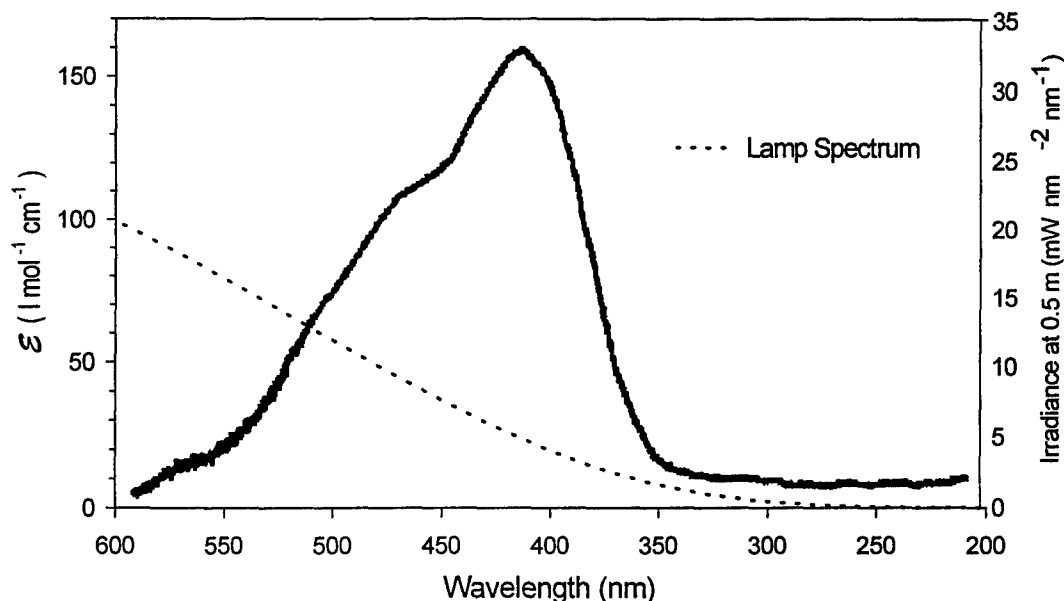


Figure 2.16 The continuous absorption spectrum of Br<sub>2</sub> (35), with lamp spectrum superimposed.

To use this equation  $I_0$  must be accurately known. In these experiments  $I_0$  was not monitored continuously, but periodic checks indicated that the intensity drifted slowly, changing very little over the time required for each individual run. If the intensity does not vary over the data-collection period the bromine concentration is

$$[Br_2] = [Br_2]_s - \frac{1}{\sigma_{Br_2} l} \ln \left( \frac{I}{I_s} \right) \quad (2.22)$$

where  $I_s$  is the transmitted light intensity when the bromine concentration is  $[Br_2]_s$ .

The value of the cross section was determined by recording the transmitted light intensity as a bromine-filled cell was slowly evacuated. Plotting the log of the light intensity (detector output in mV) versus the cell pressure yields a straight line (Figure 2.17). Equation 2.23 shows that the cross section can be determined from the slope of the line if the absorption path length is known and Equation 2.5 is used

to convert the pressure to a concentration.

$$\ln I = -(\sigma_{Br_2} [Br_2] l) + \ln I_0 \quad (2.23)$$

Figure 2.17 includes the data from two runs, one for the cell with  $\text{CaF}_2$  windows and one for the shorter cell with Pyrex windows. The two curves were forced to coincide at  $P = 0$ ; the light intensity varied between these runs because Pyrex and calcium fluoride transmit different fractions of the light at 409 nm and because the apparatus geometry changed. For the cell with  $\text{CaF}_2$  windows this technique gives

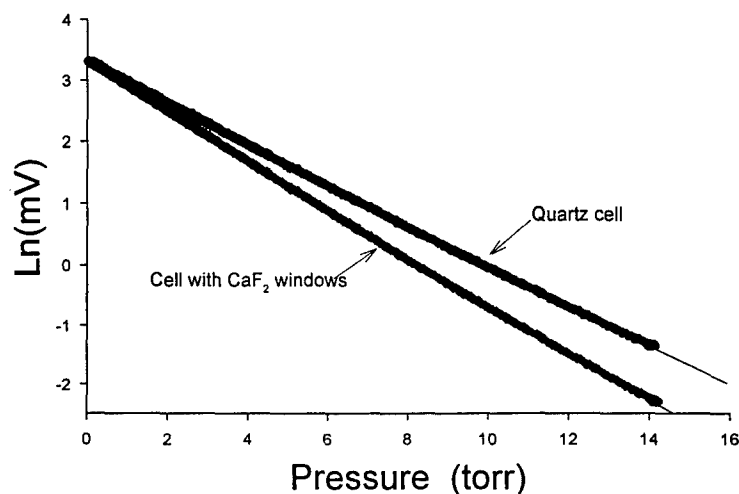


Figure 2.17 Natural log of the transmitted light intensity at 409 nm versus  $\text{Br}_2$  pressure, for 20 cm long cell with  $\text{CaF}_2$  windows and 18 cm long cell with Pyrex windows, with linear fits to data.

an average value for the slope of the intensity versus pressure data of  $.393 \pm .006$  torr $^{-1}$ . Since the pressure measured while the shutter is open is the sum of the Br pressure and the  $\text{Br}_2$  pressure, the actual partial pressure of bromine that should be used in this calculation is slightly less than the measured total pressure. Although the correction depends on how much of the bromine is dissociated and therefore varies with the light intensity and possibly the pressure, the linearity of the data in Figure

2.20 indicates that the correction for pressures below 15 torr is nearly constant. At these pressures approximately 2.2% of the bromine is dissociated (Figure 2.20) yielding a corrected value for the slope of  $.411 \pm .006 \text{ torr}^{-1}$ . The absorption path length is  $20 \pm .1 \text{ cm}$ , and using Equation 2.5 with  $T = 293\text{K}$  the cross section is  $6.33 \pm .12 \times 10^{-19} \text{ cm}^2$ , which compares favorably with the value of  $6.30 \pm 0.54 \times 10^{-19} \text{ cm}^2$  at 409 nm obtained by Johnson (35) using essentially the same technique. Other workers (60) have reported that  $\sigma$  is  $6.25 \times 10^{-19} \text{ cm}^2$  at 409 nm. The shorter cell gave a corrected value for the slope of  $.373 \pm .007 \text{ torr}^{-1}$ , corresponding to its length of about 18 cm.

By Equation 2.5, the cell pressure just before the shutter opens is

$$P_0^T = 1.0356 \times 10^{-19} [Br_2]_0 T_0 \quad (2.24)$$

where  $T_0$  is the temperature of the gas in Kelvins and the cell pressure is in torr. If the temperature of the gas does not change after the shutter opens the total pressure is, by Equation 2.18

$$P_{calc}^T = 2P_0^T - 1.0356 \times 10^{-19} [Br_2] T_0 \quad (2.25)$$

where  $[Br_2]$  is determined from the transmitted light intensity using Equation 2.21 or Equation 2.22. The calculated change in the total pressure is

$$\Delta P_{calc}^T = P_0^T - 1.0356 \times 10^{-19} [Br_2] T_0 \quad (2.26)$$

If the gas temperature does change after the shutter opens the calculated and measured pressures will not agree. The pressure measured by the manometer is

$$P_{obs}^T = \frac{P_{calc}^T T}{T_0} \quad (2.27)$$

and the temperature change is

$$\Delta T = T_0 \left( \frac{P_{obs}^T - P_{calc}^T}{P_{calc}^T} \right) \quad (2.28)$$

Figure 2.18 compares the total pressure calculated from the transmitted light intensity using Equation 2.21 and Equation 2.26 with  $T_0 = 293\text{K}$  to the data of Figure 2.15. In this example the measured and calculated pressures agree, indicating that the gas temperature does not rise over the 10 seconds shown in this figure. Monitoring the pressure for longer times shows a small temperature rise that is probably due to a gradual increase in the temperature of the cell windows and walls. These temperature effects are discussed more fully in Section 2.6.4.

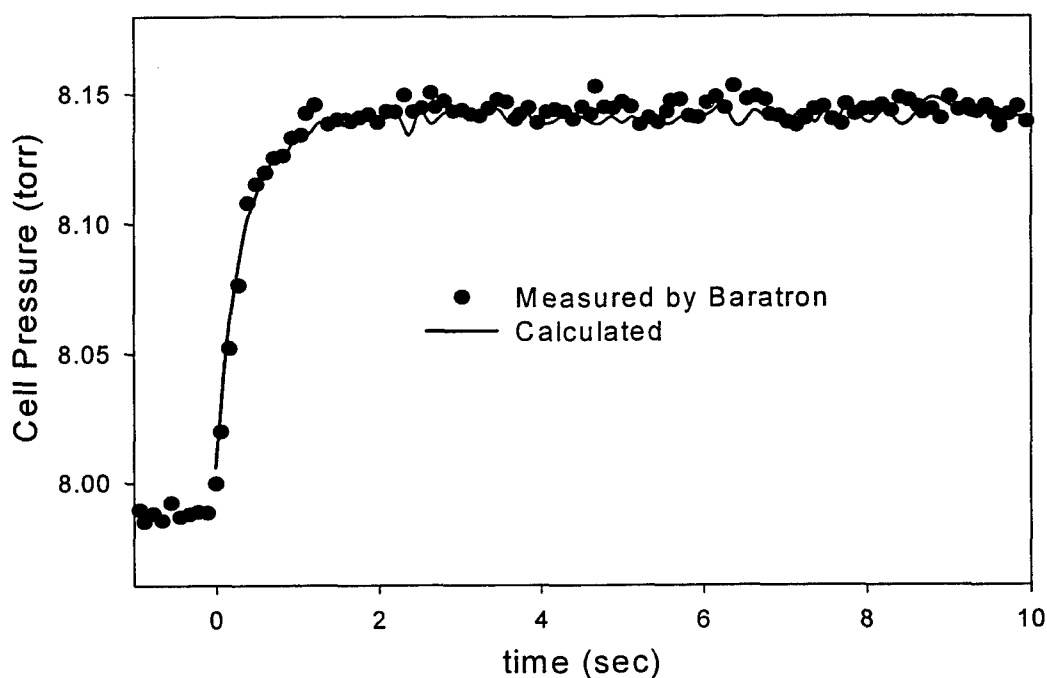


Figure 2.18 Comparison of cell pressure measured by manometer and pressure calculated from transmitted light intensity when 7.9 torr of  $\text{Br}_2$  is illuminated, at  $T_0 = 293\text{K}$ .

2.6.3 *Bromine Photolysis and Recombination.* The steady-state pressure increase rises linearly with light intensity as shown in Figure 2.19. The pressure

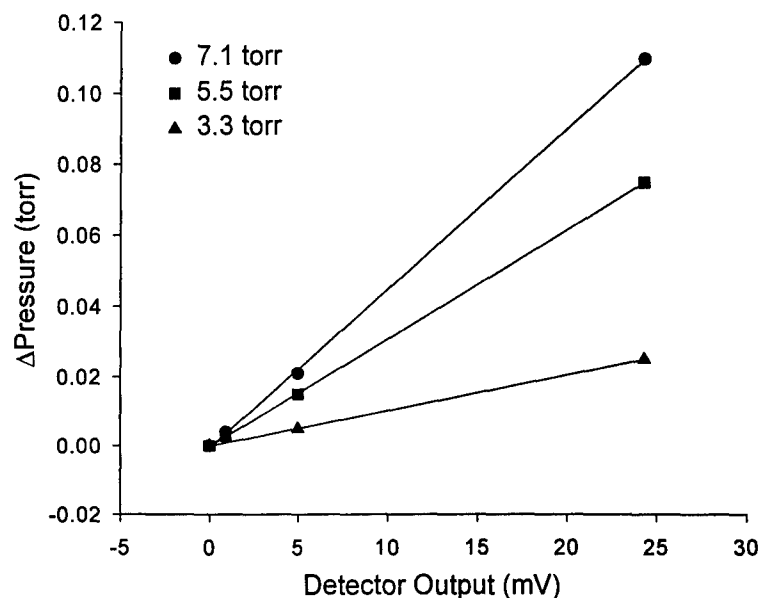
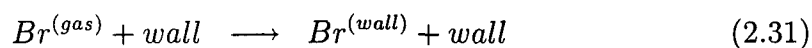
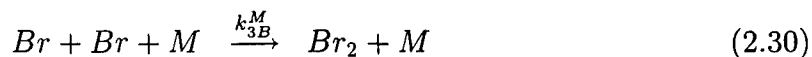
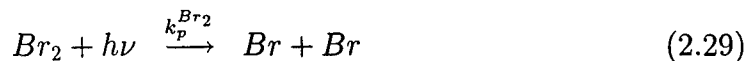


Figure 2.19 Cell pressure rise when only  $\text{Br}_2$  is in cell vs. incident light intensity. Neutral density filters used to vary light intensity.

rise (Figure 2.20) is almost constant at low pressures, then increases somewhat as the  $\text{Br}_2$  pressure rises to about 20 torr. The fraction of  $\text{Br}_2$  dissociated depends weakly on the  $\text{Br}_2$  pressure.

These observations are consistent with recent work by Johnson at AFIT (35) showing that the photodissociation of 10 torr or less of  $\text{Br}_2$  is balanced by  $\text{Br}$  atom recombination at the cell walls. At higher  $\text{Br}_2$  concentrations three-body recombination can become important, so the reactions governing the pressure rise are



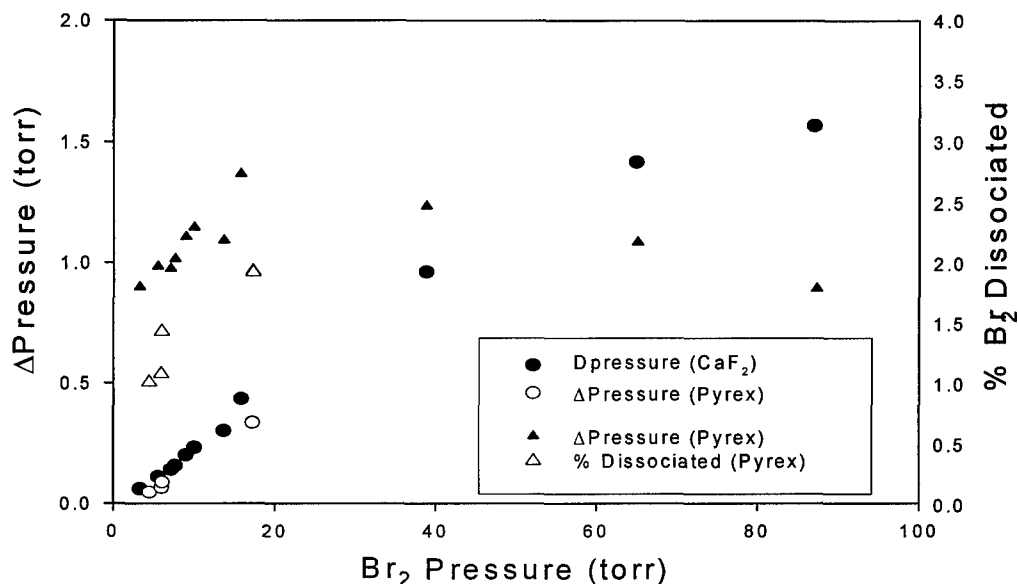


Figure 2.20 Cell pressure rise and percentage of Br<sub>2</sub> dissociated versus initial Br<sub>2</sub> pressure with only Br<sub>2</sub> in cell, using cell with CaF<sub>2</sub> windows and cell with Pyrex windows.

where M may be bromine molecules or atoms or an added inert gas. The two-step wall recombination process is equivalent to a single step in which two bromine atoms recombine to produce Br<sub>2</sub> at a rate that is proportional to the bromine atom concentration with the rate constant  $k_{obs}$ , given by

$$\frac{1}{k_{obs}} = \frac{1}{k_w} + \frac{[M]}{k_{diff}} \quad (2.33)$$

for the cylindrical geometry used here. The first term is constant at a given temperature and cell size and the second accounts for the reduction in the observed rate as higher concentrations of the species M increase the average time required for a bromine atom to diffuse to the cell wall.

The number of photodissociations per unit time per unit volume is given by the product of three factors: a wavelength-dependent pump rate coefficient  $k_p$  (cm<sup>2</sup> watt<sup>-1</sup> s<sup>-1</sup>), the intensity of the light ( $I_p$ , watts cm<sup>-2</sup>) and the concentration



(molecules  $\text{cm}^{-3}$ ) of the molecule being dissociated. When a broadband light source is used the pump rate and  $I_p$  are averages over the wavelengths responsible for the dissociation. The time rate of change of  $[\text{Br}_2]$  and  $[\text{Br}]$  are then

$$\frac{d[\text{Br}_2]}{dt} = -k_p^{Br_2} I_p [\text{Br}_2] + k_{obs}[\text{Br}] + [\text{Br}]^2 \sum k_{3B}^M[M] \quad (2.34)$$

$$\frac{d[\text{Br}]}{dt} = -2 \frac{d[\text{Br}_2]}{dt} \quad (2.35)$$

For sufficiently low pressures both the three-body recombination processes and the diffusive effects are unimportant. Under these conditions equating the time derivative of the bromine atom concentration to zero provides the ratio of  $[\text{Br}]$  to  $[\text{Br}_2]$  in steady-state as

$$\frac{[\text{Br}]_{ss}}{[\text{Br}_2]_{ss}} = \frac{k_p^{Br_2} I_p}{k_w} \quad (2.36)$$

If the number of bromine atoms attached to the wall does not change, the  $\text{Br}$  and  $\text{Br}_2$  concentrations are related to the initial bromine concentration by Equation 2.17 and the steady-state ratios of the atomic and molecular bromine concentrations to the initial bromine concentration are

$$\frac{[\text{Br}]_{ss}}{[\text{Br}_2]_0} = \frac{2 k_p^{Br_2} I_p}{2 k_w + k_p^{Br_2} I_p} \quad (2.37)$$

$$\frac{[\text{Br}_2]_{ss}}{[\text{Br}_2]_0} = \frac{2 k_w}{2 k_w + k_p^{Br_2} I_p} \quad (2.38)$$

The bromine atom concentration and the pressure rise at steady state increase linearly with the initial bromine concentration and, as long as  $k_w$  is much larger than  $k_p^{Br_2} I_p$ , linearly with the light intensity.

At intermediate bromine concentrations the pressure-dependence of the wall recombination rate must be considered. When only bromine is present the bromine

atom concentration at steady state is

$$[Br]_{SS} = k_p^{Br_2} I_p \left\{ \frac{[Br_2]}{k_w} + \frac{[Br_2]^2}{k_{diff}} \right\} \quad (2.39)$$

and the bromine atom concentration increases quadratically with  $[Br_2]$ . If  $[M]$  is something other than bromine the bromine atom concentration is

$$[Br]_{SS} = k_p^{Br_2} I_p [Br_2] \left\{ \frac{1}{k_w} + \frac{[M]}{k_{diff}} \right\} \quad (2.40)$$

and the Br concentration varies linearly with both  $[Br_2]$  and  $[M]$ . Figure 2.21 shows that adding argon to a cell filled with bromine increases the pressure rise when the light is turned on. The pressure change after the argon is added can be used to

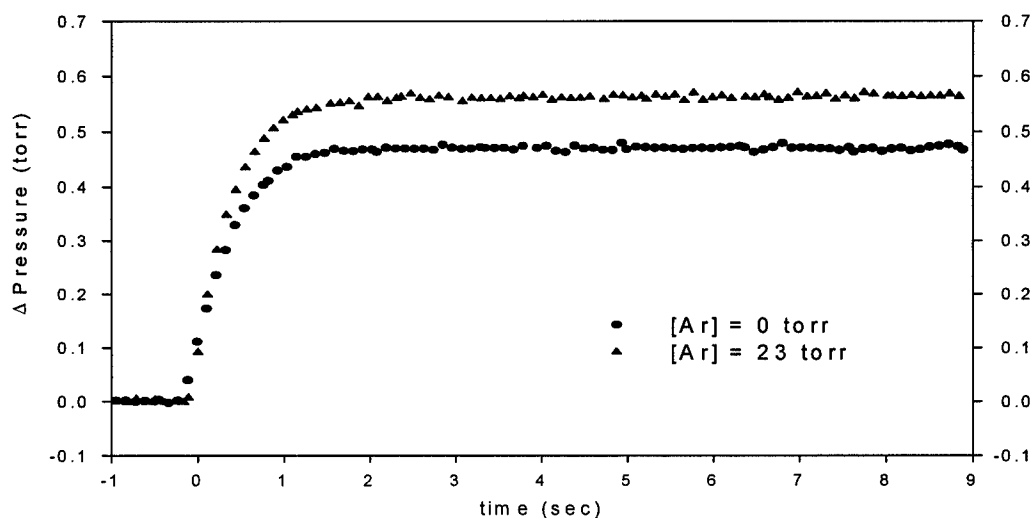


Figure 2.21 An example showing that adding 23 torr of argon to 19.81 torr of bromine increases the pressure rise when the mixture is illuminated.

estimate the relative values of  $1/k_w$  and  $[Ar]/k_{diff}$ . Equations 2.40 and 2.19 give

$$\begin{aligned} \Delta P_2 - \Delta P_1 &\approx \frac{k_p^{Br_2} I_p P_0(Br_2) P(Ar)}{2 k_{diff}} \\ .1 \text{ torr} &\approx \frac{k_p^{Br_2} I_p \times 19.81 \text{ torr} \times 23 \text{ torr}}{2 k_{diff}} \end{aligned}$$

$$\frac{k_p^{Br_2} I_p}{k_{diff}} \approx .00044 \text{ torr}^{-1}$$

This makes  $[Ar]/k_{diff}$  larger than  $1/k_w$  for argon pressures above about 90 torr. Johnson (35) reported values of  $131 \text{ s}^{-1}$  for  $k_w$  and  $382 \text{ torr s}^{-1}$  for  $k_{diff}$  when 0 to 100 torr of argon was added to 2 torr of bromine; for his experiment  $[Ar]/k_{diff}$  was larger than  $1/k_w$  for  $[Ar]$  above about 3 torr. The two experiments cannot be compared directly, however, for three reasons. Firstly, the radii of the cells used in the two experiments were different and  $k_{diff}$  varies as  $r^{-2}$ . Secondly, Johnson used a laser to dissociate the bromine molecules in a small volume at the axis of his cell so each bromine atom had to travel a distance equal to approximately the radius of the cell before recombining at the wall; in this experiment the entire cell volume was illuminated and the minimum distance to the wall varied. To first order this difference affects only the value of the diffusion constant in Equation 2.33, leaving the general form of the dependence on  $[M]$  unchanged (54). Finally, the original bromine concentration used here was almost ten times the bromine concentration Johnson used.

When three-body recombination is ignored Equations 2.35 and 2.19 give

$$\begin{aligned} \Delta P &= \frac{k_p^{Br_2} I_p P_0(Br_2)}{k_p^{Br_2} I_p + 2 k_{obs}} \left\{ 1 - \exp[-(k_p^{Br_2} I_p + 2 k_{obs}) t] \right\} \\ &= P_0(Br_2) a \left\{ 1 - \exp[-b (t - c)] \right\} \end{aligned} \quad (2.41)$$

The fit parameter  $c$  is added to account for any inaccuracy in the determination of  $t = 0$  and to compensate for the effect of the short but non-zero time required for the shutter to fully open. In Figures 2.22 and 2.23 Equation 2.41 is fit to pressure rise data for the long and short cells. The initial bromine pressures and the results of the fits are given in Table 2.4.

The variation in  $k_p I_p$  is due to several factors. The incident light intensity varied somewhat due to differing apparatus configurations. In addition to this,  $k_p I_p$

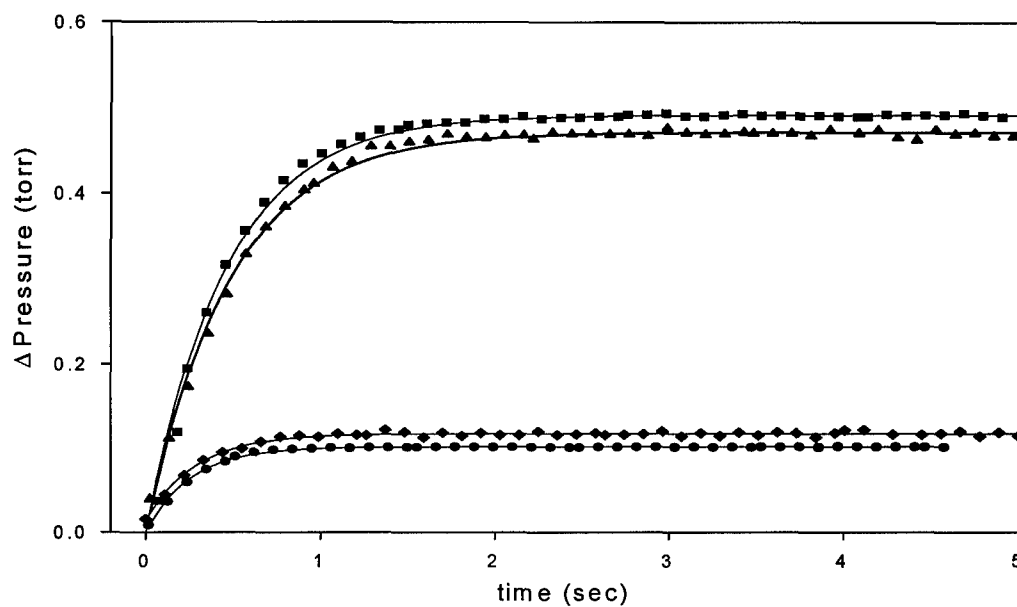


Figure 2.22 Fits to the cell pressure rise for several initial  $\text{Br}_2$  pressures, using 20 cm long cell with  $\text{CaF}_2$  windows. (See Table 2.4)

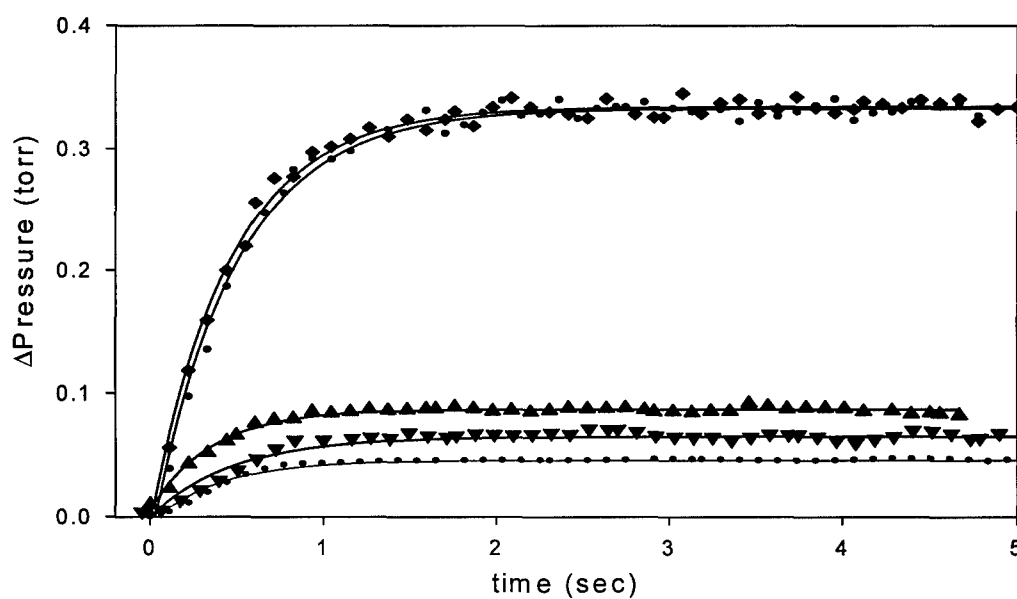


Figure 2.23 Fits to the cell pressure rise for several initial  $\text{Br}_2$  pressures, using 18 cm long cell with Pyrex windows. (See Table 2.4)

Table 2.4 Results of fits to pressure rise data.

$P_0(\text{Br}_2)$ (torr)	a	b ( $\text{s}^{-1}$ )	$k_p^{\text{Br}_2} I_p$ ( $\text{s}^{-1}$ )	$k_{obs}$ ( $\text{s}^{-1}$ )
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20 cm long cell with  $\text{CaF}_2$  windows

5.90	.0198	3.492	.069	1.711
7.12	.0143	3.906	.056	1.925
17.67	.0278	2.208	.061	1.073
19.81	.0238	2.101	.050	1.026

18 cm long cell with Pyrex windows

4.50	.0102	2.573	.026	1.273
5.98	.0109	2.107	.023	1.042
9.82				1.160
6.07	.0144	2.812	.040	1.386
17.27	.0194	2.151	.042	1.055
17.28	.0193	2.058	.040	1.009

drops as the bromine concentration increases because it is an average over the length of the cell and the light intensity decreases more quickly with distance at higher bromine concentrations. The two examples in the short cell which have  $k_p^{\text{Br}_2} I_p$  values of about  $0.025 \text{ s}^{-1}$  are inconsistent with the other measurements. The pressure versus time plots in Figure 2.23 for these runs have initial slopes that are lower than that those predicted by the model and are shaped differently.

The value of  $k_p I_p$  does not affect the values of  $k_w$  and  $k_{diff}$  found using Equation 2.33. A linear fit (Figure 2.24) to the long cell data gives  $k_w = 2.9 \text{ s}^{-1}$  and  $k_{diff} = 30 \text{ torr s}^{-1}$ . The two rates are equal when  $P(\text{Br}_2)$  is 10.3 torr. For the short cell the fit gives  $k_w = 1.61 \text{ s}^{-1}$  and  $k_{diff} = 49.79$  and the two rates are equal for  $P(\text{Br}_2) = 30.9 \text{ torr}$ . There is not enough data in these plots, however, to draw any firm conclusions from the fits.

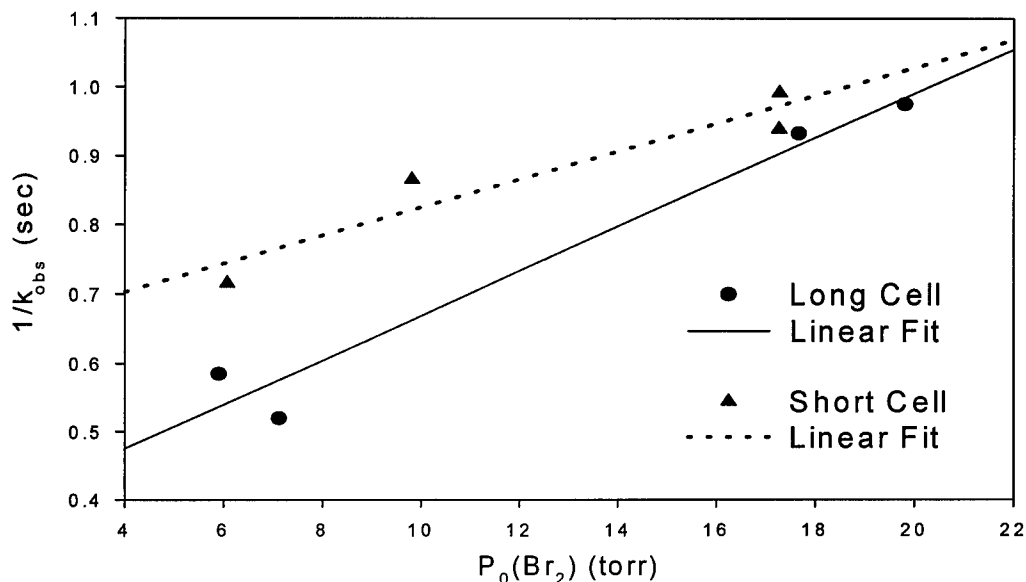


Figure 2.24 Linear fit to  $1/k_{\text{obs}}$  versus  $P_0(\text{Br}_2)$  data derived from fits to pressure rise.

At high pressures three-body recombination becomes the dominant Br recombination mechanism and the steady state bromine atom concentration is

$$[\text{Br}]_{\text{ss}} = \left( \frac{k_p^{\text{Br}_2} I_p [\text{Br}_2]}{\sum k_{3B}^M [\text{M}]} \right)^{\frac{1}{2}} \quad (2.42)$$

The details of the variation of the bromine atom concentration with pressure depend on the concentrations and the relative efficiencies of the various species that act as the third body in the recombination process. Ip and Burns (33) reported rate constants at 300K for  $\text{Br}_2$  as the third body of  $32$  to  $1600 \text{ torr}^{-2}\text{s}^{-1}$  and for Br of  $46$  to  $460,000 \text{ torr}^{-2}\text{s}^{-1}$ . When 2% of the bromine is dissociated, the rates of Br recombination with Br and  $\text{Br}_2$  as the third bodies are equal when the rate constant for Br is about 25 times as large as that for  $\text{Br}_2$ , well within the error bounds on the Br rate constant. Baulch (4), however, reports that the rate constant for Br is only about 10 times that of  $\text{Br}_2$ .

With only bromine in the cell the dependence of the bromine atom concentration on initial  $\text{Br}_2$  pressure falls between two extremes. If the influence of Br atoms can be ignored the steady-state bromine atom concentration depends only on the light intensity:

$$[\text{Br}]_{ss} = \left( \frac{k_p^{\text{Br}_2} I_p}{k_{3B}^{\text{Br}_2}} \right)^{\frac{1}{2}} \quad (2.43)$$

and the fraction of bromine dissociated drops as the inverse of the bromine pressure. If the bromine molecules can be ignored, the Br concentration is

$$[\text{Br}]_{ss} = \left( \frac{k_p^{\text{Br}_2} I_p [\text{Br}_2]}{k_{3B}^{\text{Br}_2}} \right)^{\frac{1}{3}} \quad (2.44)$$

and the fraction dissociated decreases as  $[\text{Br}_2]^{-2/3}$ . The decrease in the fraction of bromine dissociated seen in Figure 2.20 for initial bromine pressures larger than about 20 torr indicates that three-body recombination of Br atoms becomes important at these pressures, since only when three-body recombination is important does the fraction of bromine dissociated decrease with increasing bromine pressure. However, the bromine concentration is still increasing even at 100 torr, indicating that three-body recombination mediated by  $\text{Br}_2$  is not the dominant recombination mechanism at that pressure. Johnson found that the three-body recombination of bromine atoms could be ignored at argon pressures as high as 100 torr; Ip and Burns determined that the rate constant for argon is 6.63 to 7.12 torr<sup>-2</sup>s<sup>-1</sup>, so argon acts much less efficiently than Br or  $\text{Br}_2$  as the third body.

*2.6.4 Distribution of Excess Photon Energy after  $\text{Br}_2$  Dissociation.* When a  $\text{Br}_2$  molecule is dissociated, the photon energy in excess of that required to break the Br-Br bond is divided between the two resulting bromine atoms. The dissociation energy of  $\text{Br}_2$  is 1.968 eV, equaling the energy of a 630 nm photon (35). A rough estimate based on Figure 2.16 indicates that the average excess energy after dissociation is about .75 eV. With  $k_p^{\text{Br}_2} I_p = .05 \text{ s}^{-1}$  and  $P(\text{Br}_2) = 15 \text{ torr}$  at 293K

there are about  $2.5 \times 10^{16}$  dissociations per second per  $\text{cm}^3$ . The cell volume is  $360 \text{ cm}^3$  so if all of the excess energy immediately heats the gas the thermal energy of the gas increases by about 1 J per second. The molar heat capacity of  $\text{Br}_2$  at 293K is 28 J/mol-K (38) and fifteen torr of bromine in  $360 \text{ cm}^3$  is .0003 moles. The temperature would rise 120K per second. The lack of any significant heating effect after the shutter opens indicates that the excess energy does not increase the average kinetic energy of the bulk of the molecules in the cell.

Although the bromine atoms cannot possess vibrational or rotational energy, the excess energy may appear as electronic as well as translational energy. If the incident wavelength is less than approximately 430 nm two ground state  $\text{Br}(^2\text{P}_{3/2})$  atoms are formed but for wavelengths between 430 and 510.6 nm nearly equal proportions of ground state and excited  $\text{Br}(^2\text{P}_{1/2})$  atoms are formed (35). The electronically excited  $\text{Br}^*$  state is 0.456 eV above the ground state. The quantum yield drops from 85% at 510 nm to 12% at 550 nm. (A quantum yield of 100% corresponds to the production of one  $\text{Br}^*$  atom and one ground state atom for every absorbed photon.) Figure 2.25 shows the quantum yield for  $\text{Br}(^2\text{P}_{1/2})$  production as a function of the wavelength of the dissociating light and Figure 2.26 shows the sections of the  $\text{Br}_2$  absorption curve corresponding to the different upper levels accessed by the excited bromine molecule before it dissociates. Figure 2.16 indicates that a large fraction of the bromine atoms produced in this experiment are excited, significantly reducing the fraction of the excess energy that immediately appears as kinetic energy of the bromine atoms. The excited bromine atoms are deactivated by collisions with bromine molecules. The rate for this process is  $1.2 \pm 0.1 \times 10^{-12} \text{ cm}^3/\text{molecule-s}$  (35). If half of the bromine atoms produced by dissociation are in the excited electronic state the production rate is balanced by the deactivation rate when  $[\text{Br}^*] = 4.2 \times 10^{10} \text{ atoms/cm}^3$  or  $1.3 \times 10^{-6} \text{ torr}$  at 293K. Very little of the excess photon energy, therefore, is tied up as  $\text{Br}^*$  electronic energy. When the excited bromine



atoms collide with bromine molecules the electronic energy is transferred primarily into  $\text{Br}_2$  vibrational energy.

The molecular vibrational energy is eventually transformed into kinetic energy, but this may not happen until the bromine molecule strikes the cell wall. Additionally, at the pressures used in these experiments bromine atom recombination occurs mainly at the cell walls. If the bromine atoms have not lost the excess kinetic energy they had immediately after their formation that energy will also be transferred to the cell and not to the bromine molecules. The heat capacity of the cell is large enough that its temperature rises only slowly as the kinetic energy is deposited.

In Section 2.7.4 the absence of a significant heating effect when  $\text{Br}_2$  is dissociated is contrasted with the temperature increase of a mixture of  $\text{Br}_2$ ,  $\text{BrNO}$  and  $\text{NO}$  when the shutter is opened.

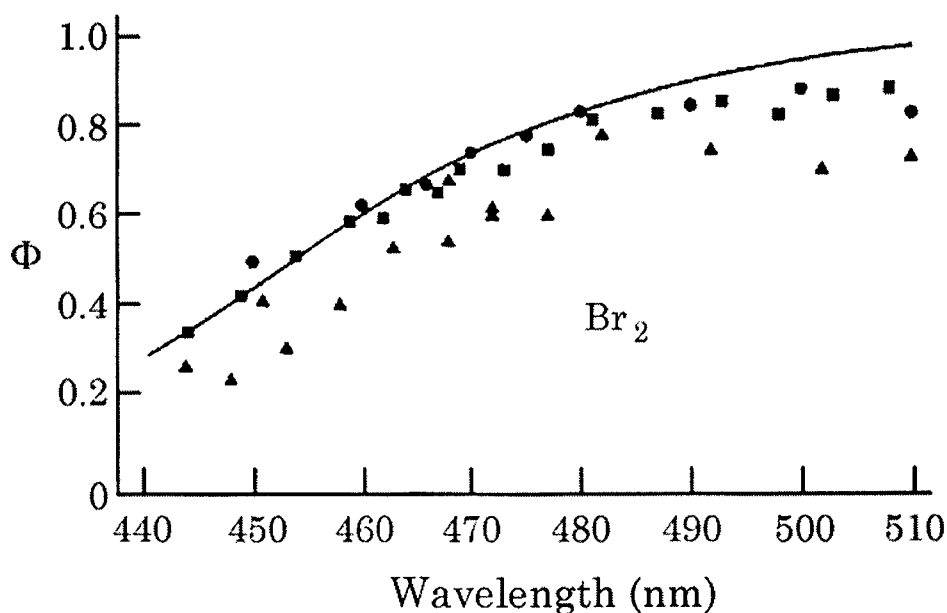


Figure 2.25 Quantum yields of  $\text{Br}^*$  production from  $\text{Br}_2$  photolysis as a function of wavelength. The symbols represent experimental data and the solid curve represents a theoretical calculation (26).

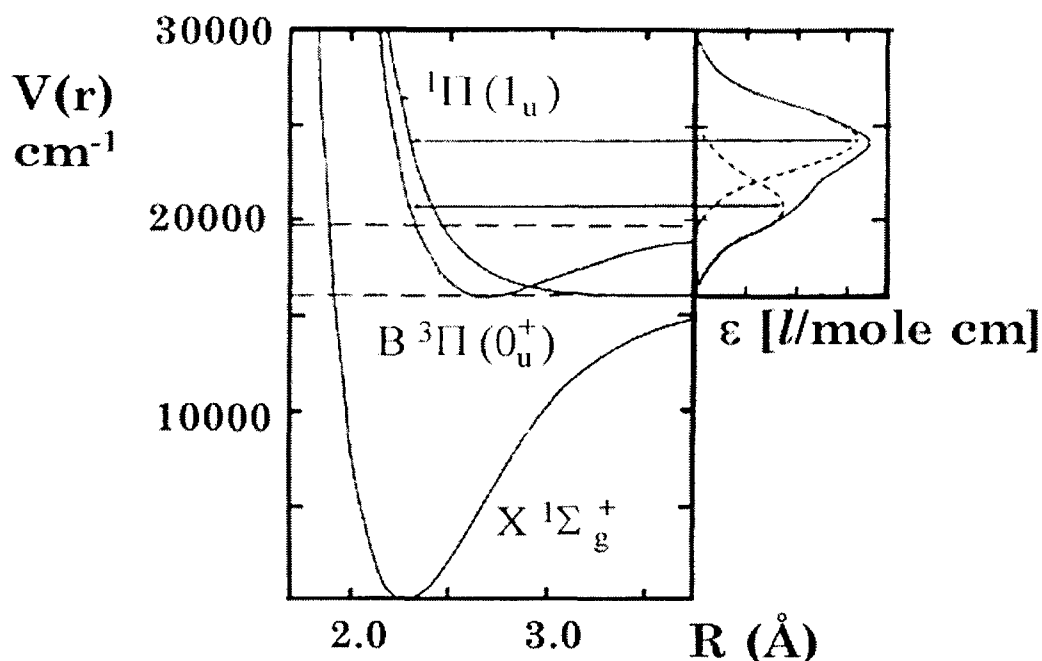


Figure 2.26  $\text{Br}_2$  potential energy curves (49).

*2.6.5 Summary.* In this section the bromine absorption coefficient was found to agree with the values reported by other workers. This, combined with the analysis of the dissociation and recombination of bromine, demonstrates that the apparatus used in these experiments provides reproducible, reliable data. The information obtained in these preliminary sections is used in the next sections to analyze the kinetics of a mixture of NO,  $\text{Br}_2$  and BrNO exposed to light.

## *2.7 Reactions when NO and BrNO are Present*

The goal of this section is to develop a model that explains what happens when an equilibrated mixture of NO,  $\text{Br}_2$  and BrNO is illuminated. Like bromine, BrNO can be photodissociated if illuminated with light energetic enough to break one or more of the bonds holding the molecule together. The most common type of

photodissociation for triatomic molecules is (49)



where the X-Y bond is weaker than the Y-Z bond. The N-O bond in BrNO is much stronger than the Br-N bond so photodissociation produces a Br atom and an NO molecule.

Figure 2.27 illustrates the temporal behavior of the cell pressure after the shutter opens. There is a sudden pressure jump followed by a slower increase that eventually reaches a near photo-stationary state. When the light is turned off, the pressure drops quickly by an amount that is slightly less than the initial prompt rise, then slowly approaches its final pressure. These features are present whenever an equilibrated mixture is illuminated but the magnitudes and slopes of the pressure changes depend on the initial pressures and the light intensity.

*2.7.1 BrNO Absorption Cross Section.* As in the bromine-only case, monitoring the transmitted light intensity allows any temperature effects to be identified. The bond energy of NO corresponds to a wavelength of 190.8 nm, but NO begins to absorb at about 230 nm (49). It is not dissociated and does not absorb light at the wavelengths emitted by the Oriel lamp. Nitrosyl bromide does absorb at these wavelengths (Figure 2.28), making the transmitted light intensity a function of the concentrations of BrNO and Br<sub>2</sub>. The transmitted light intensity if only NO, BrNO and Br<sub>2</sub> molecules and Br atoms are present is

$$I = I_0 \exp\{ -(\sigma_{Br_2}[Br_2] + \sigma_{BrNO}[BrNO]) l \} \quad (2.46)$$

The value of  $\sigma_{BrNO}$  is slightly more difficult to determine than that of  $\sigma_{Br_2}$  since BrNO is inevitably accompanied by Br<sub>2</sub>. By mixing a small amount of Br<sub>2</sub> with a large excess of NO, however, the amount of Br<sub>2</sub> in the cell before the shutter is

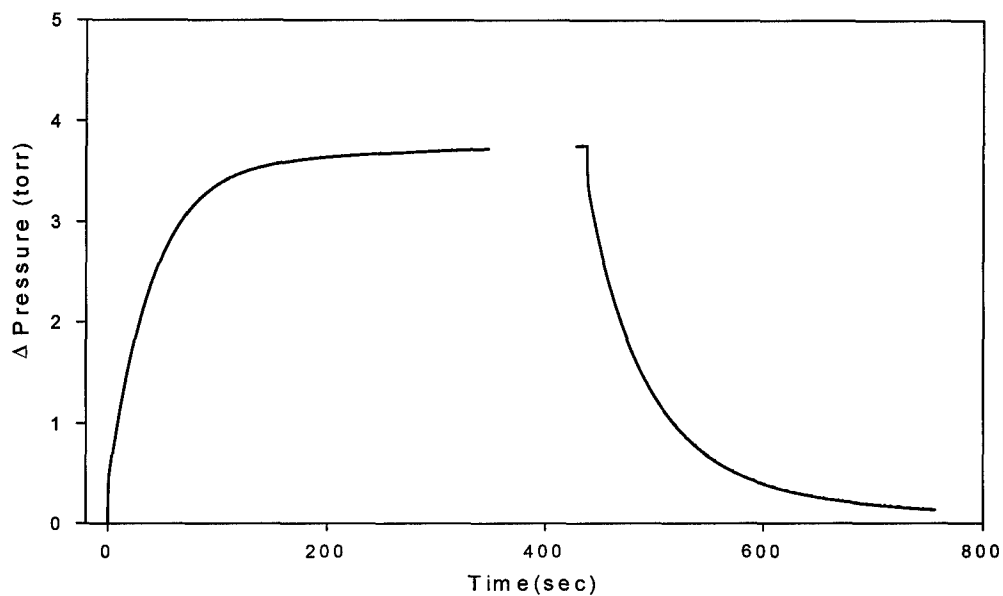


Figure 2.27 Example of cell pressure change when equilibrated mixture of NO, BrNO and Br<sub>2</sub> is illuminated. When the shutter opened the cell contained 52.6 torr NO, .1 torr Br<sub>2</sub> and 7.6 torr BrNO.

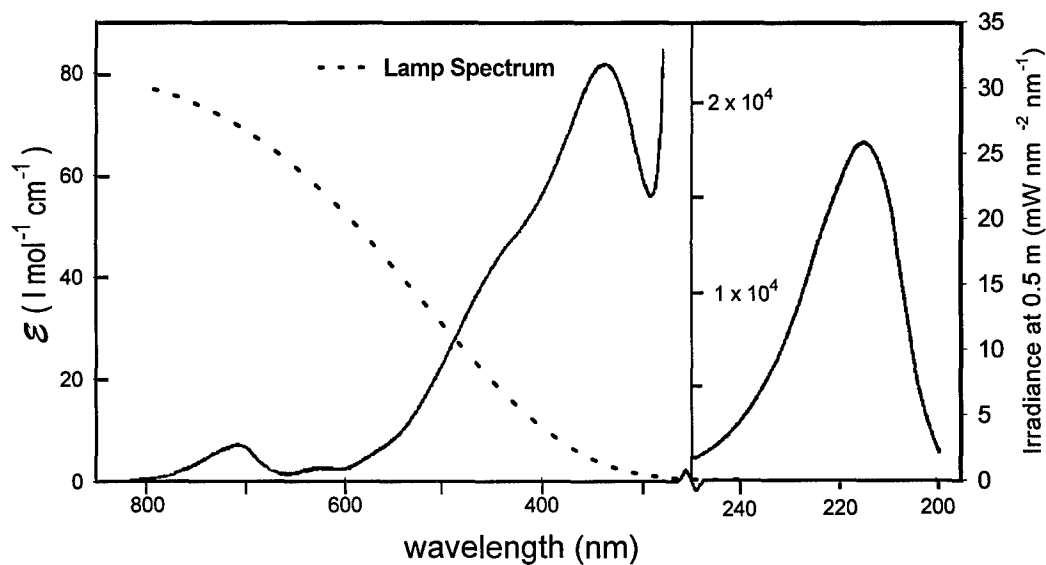


Figure 2.28 The ultraviolet/visible absorption spectrum of BrNO at  $300 \pm 3$  K, from Houel (32).

opened can be minimized. When 150 torr of NO is added to 7.5 torr of Br<sub>2</sub>, for instance, 99.3% of the bromine is converted to BrNO. Illuminating the mixture does not change the concentrations. (Under these conditions no correction for BrNO dissociation is required. See Section 2.7.3 and Figure 2.43.) Any absorption of the light passing through the cell must then be due almost entirely to BrNO and the small contribution from Br<sub>2</sub> can be ignored. This technique yields a value for  $\sigma_{BrNO}$  of  $2.02 \pm .027 \times 10^{-19} \text{ cm}^2$ . The value of the cross section determined from Houel's absorption curve (Figure 2.28) is about .35 times that of bromine, or  $2.2 \times 10^{-19} \text{ cm}^2$ . Houel noted that the measured value of the cross section was independent of the resolution of the detector for  $0.2 \leq \Delta\lambda(\text{FWHM}) \leq 2 \text{ nm}$ . The relatively wide bandpass ( $10 \pm 2 \text{ nm}$ ) of the 409 nm filter used in the experiments reported here will therefore affect the measured value of the cross section and explains the 8% difference between the present experimental value and Houel's result. Houel also reported that the BrNO absorption cross section changes very little with temperature.

Figures 2.29 and 2.30 demonstrate that the lamp output between 450 and 850 nm is primarily responsible for the pressure rise seen when a mixture of Br<sub>2</sub>, NO and BrNO is illuminated. Below 450 nm the lamp output is very weak and above 800 nm the absorption coefficients of both Br<sub>2</sub> and BrNO are negligible. The data in these plots cannot be compared quantitatively because the passband transmittancies of each filter varied. If the 850 nm short-pass filter passed all of the light at wavelengths less than 850 nm the pressure rise with the filter in place would match that when no filter is used, but in Figure 2.30 the pressure rise with the 850 nm short-pass filter in place is significantly less than that when no filter is used. The transmitted light intensity at 409 nm when the 850 nm short-pass filter is in place is only .003 times the intensity when no filter is used, however, indicating that the passband of the filter does not extend far enough to cover all of the lamp output below 850 nm.

*2.7.2 Experimental Procedure.* In these experiments NO and Br<sub>2</sub> were mixed as for the dark reaction studies and allowed to approach equilibrium. The time

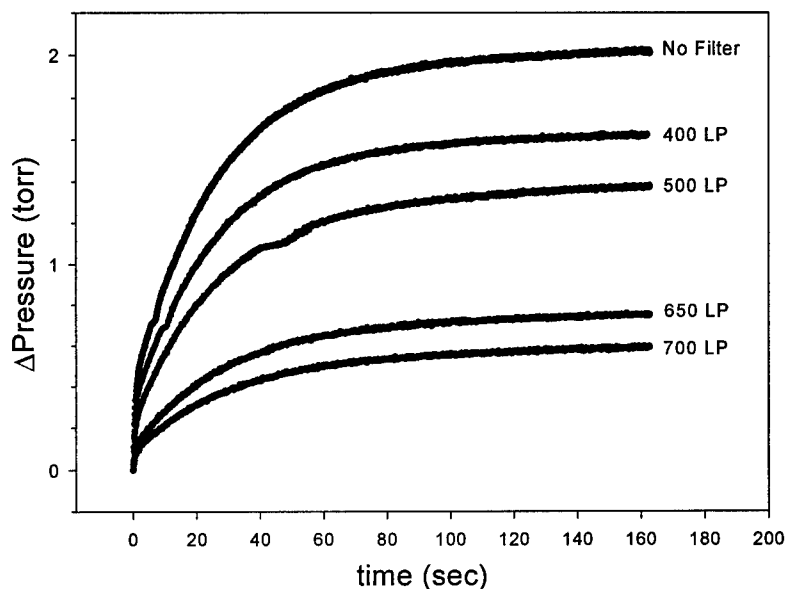
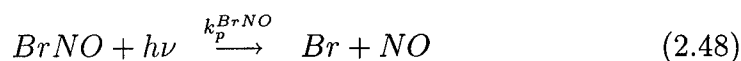
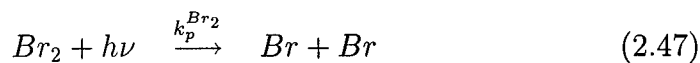


Figure 2.29 Pressure rise with several long-pass filters placed between the lamp and the cell.  $P_0(\text{Br}_2) = .36$  torr,  $P_0(\text{NO}) = 40.55$  torr,  $P_0(\text{BrNO}) = 21.2$  torr.

required for each mixture to proceed 99.5% of the way to equilibrium (Figure 2.31) was calculated using the previously determined rate constants and the shutter opened after at least this much time had elapsed.

**2.7.3 Mechanism.** While there are a number of reactions that might occur when a mixture of  $\text{Br}_2$ ,  $\text{NO}$  and  $\text{BrNO}$  is illuminated, the goal is to determine a minimum set of reactions that explains the observations. The bromine-only work suggests that wall recombination and three-body recombination of bromine atoms may be important. Previous work has shown that bromine atoms react with  $\text{BrNO}$  to form  $\text{Br}_2$  and  $\text{NO}$ , providing another mechanism that reduces the bromine atom concentration. A possible kinetic mechanism, then, is



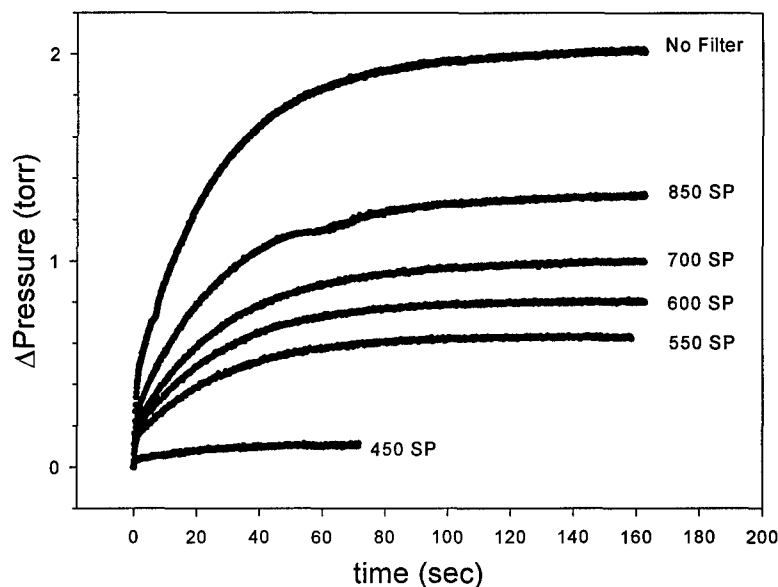
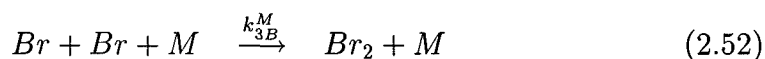
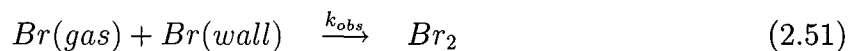
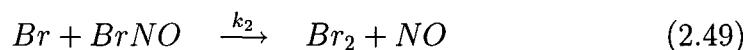


Figure 2.30 Pressure rise with several short-pass filters placed between the lamp and the cell.  $P_0(\text{Br}_2) = .36$  torr,  $P_0(\text{NO}) = 40.55$  torr,  $P_0(\text{BrNO}) = 21.2$  torr.



Reactions 2.51 and 2.52 are the same bromine atom recombination mechanisms discussed in Section 2.6.1. The resulting rate equations for the concentrations of  $\text{Br}_2$ ,  $\text{NO}$ ,  $\text{BrNO}$  and  $\text{Br}$  are:

$$\begin{aligned} \frac{d[\text{Br}]}{dt} = & 2k_p^{\text{Br}_2} I_p[\text{Br}_2] + k_p^{\text{BrNO}} I_p[\text{BrNO}] - k_2[\text{Br}][\text{BrNO}] \\ & - 2k_{\text{obs}}[\text{Br}] - 2[\text{Br}]^2 \sum k_{3B}^M[\text{M}] \end{aligned} \quad (2.53)$$

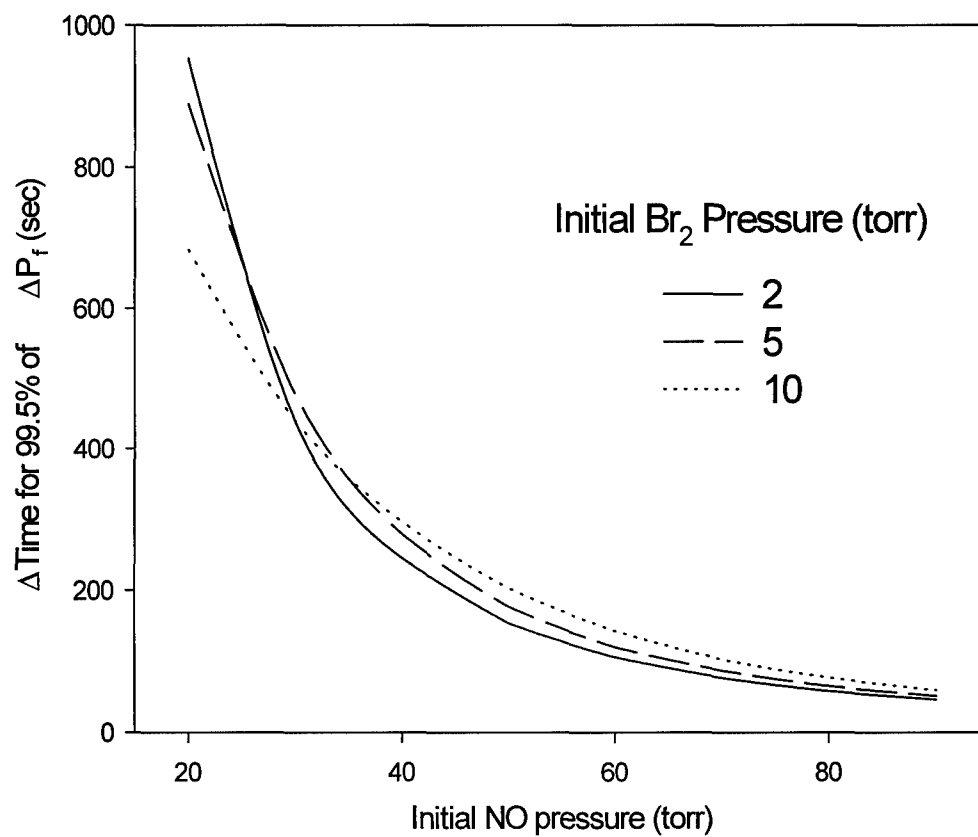


Figure 2.31 Time required for dark reactions to reach 99.5% of final pressure change, for a range of initial bromine and NO pressures.



$$\begin{aligned} \frac{d[Br_2]}{dt} = & -k_p^{Br_2} I_p[Br_2] + k_p^{BrNO} [Br][BrNO] - k_f[Br_2][NO]^2 \\ & + k_{obs}[Br] + k_r[BrNO]^2 + [Br]^2 \sum k_{3B}^M[M] \end{aligned} \quad (2.54)$$

$$\begin{aligned} \frac{d[NO]}{dt} = & k_p^{BrNO} I_p[BrNO] + k_2[Br][BrNO] - 2k_f[Br_2][NO]^2 \\ & + 2k_r[BrNO]^2 \end{aligned} \quad (2.55)$$

$$\frac{d[BrNO]}{dt} = -\frac{d[NO]}{dt} \quad (2.56)$$

Reaction (2.49) is extremely fast, with reported values of its rate constant ranging from  $7.25 \times 10^4$  to  $1.71 \times 10^5$  torr<sup>-1</sup>s<sup>-1</sup>. Table 2.5 compares the rates for the reactions listed above assuming that the same fraction of bromine molecules is dissociated as in the bromine-only experiments, about 2%, and that all the species in the gas are as efficient as bromine when participating in three-body recombinations. The total gas pressure was taken as 44 torr.

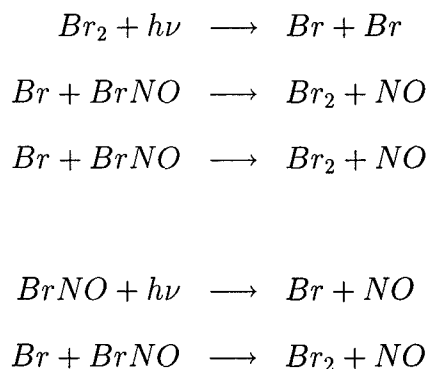
Table 2.5 Comparison of reaction rates for  $[Br_2] = 7$  torr,  $[NO] = 27$  torr, and  $[BrNO] = 10$  torr.

Reaction	Rate (torr s <sup>-1</sup> )
$Br + BrNO \longrightarrow Br_2 + NO$	$2 \times 10^5$
$Br + Br + M \longrightarrow Br_2 + M$	200
$Br(g) + Br(w) \longrightarrow Br_2$	0.4
$Br_2 + 2 NO \longrightarrow 2 BrNO$	.11
$2 BrNO \longrightarrow Br_2 + 2NO$	.0065

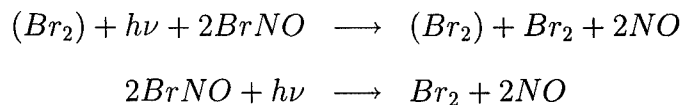
If the bromine atom concentration is controlled exclusively by reaction with BrNO, the steady-state Br atom concentration is

$$[Br]_{ss} = \frac{k_p^{BrNO} I_p}{k_2} + \frac{2k_p^{Br_2} I_p[Br_2]}{k_2[BrNO]} \quad (2.57)$$

For  $k_p^{Br_2} I_p = .055 \text{ s}^{-1}$ ,  $k_p^{BrNO} I_p = .018 \text{ s}^{-1}$ ,  $P(Br_2) = P(BrNO) = 10 \text{ torr}$  and  $k_2 = 3 \times 10^{-12} \text{ cm}^3/\text{molecule-s}$  the bromine atom concentration is  $4.5 \times 10^{10} \text{ atoms/cm}^3$ , equivalent to a pressure of  $1.3 \times 10^{-6} \text{ torr}$  at 293K. The Br concentration can become significant only if the BrNO concentration is very small. If this happens the Br recombination processes that do not require the presence of BrNO concentration will determine the Br concentration. The same mechanisms will operate as in the bromine-only case, except that now the NO molecules will affect the diffusion rate and can participate in the three-body recombination of bromine atoms. When the BrNO concentration is large enough to control the Br concentration, the bromine atoms liberated by photodissociation of  $Br_2$  and BrNO are immediately converted into  $Br_2$  and NO:



These reactions sum to give



The photolysis of BrNO in conjunction with the reaction of Br atoms with BrNO result in the destruction of BrNO with a quantum yield of 2. This has been observed for the photodissociation of ClNO (49). Additionally, the dissociation of  $Br_2$  and BrNO ultimately produce concentration changes that mimic the reverse reaction in

Equation 2.1. The effect of dissociation therefore is to shift the equilibrium between  $\text{Br}_2$ ,  $\text{NO}$  and  $\text{BrNO}$  that was established before the shutter opened towards more  $\text{Br}_2$  and  $\text{NO}$ . The resulting time derivatives of the concentrations are:

$$\frac{d[\text{Br}_2]}{dt} = k_p^{\text{Br}_2} I_p [\text{Br}_2] + k_p^{\text{BrNO}} I_p [\text{BrNO}] - k_f [\text{Br}_2] [\text{NO}]^2 + k_r [\text{BrNO}]^2 \quad (2.58)$$

$$\frac{d[\text{NO}]}{dt} = 2 \frac{d[\text{Br}_2]}{dt} \quad (2.59)$$

$$\frac{d[\text{BrNO}]}{dt} = -\frac{d[\text{NO}]}{dt} \quad (2.60)$$

As long as the bromine atom concentration is small the stoichiometry of the dark reactions will be maintained and the concentrations can be expressed in terms of a progress variable  $x(t)$ . At constant temperature the pressure change is

$$\begin{aligned} P^T - P_0^T &= (P_0(\text{Br}_2) - P(x)) + (P_0(\text{NO}) - 2 P(x)) + (P_0(\text{BrNO}) + 2 P(x)) - P_0^T \\ \Delta P &= -P(x) \end{aligned}$$

and the pressure change calculated from the light intensity is

$$\Delta P_{\text{calc}} = -1.0356 \times 10^{-19} T_0 \frac{\ln I - \ln I_s}{(\sigma_{\text{Br}_2} - 2\sigma_{\text{BrNO}}) l} \quad (2.61)$$

where  $I_s$  is the light intensity when the pressure is  $P_0^T$ . Any errors in the measurement of the initial pressures and  $I_a$  shift the calculated  $\Delta P$  curve up or down but do not change its shape, which depends only on the values of  $\sigma_{\text{Br}_2}$  and  $\sigma_{\text{BrNO}}$ . If these constants are correct the calculated and observed pressure rise curves will overlay as long as the stoichiometry of the dark reactions is maintained and the temperature of the gas does not increase. The vertical shift required to overlay the two curves can be compared to the value calculated using  $I_0$  and the initial concentrations to detect any errors in these measurements.

2.7.4 *Prompt Pressure Rise.* The prompt pressure rise after the shutter opens appears similar to the pressure rise when bromine alone is dissociated, but in this case it is caused by a temperature rise and not a concentration change. In the bromine-only cases (Section 2.6.3) the  $\text{Br}_2$  concentrations calculated from the transmitted light intensity and from the pressure rise agreed, indicating that little of the pressure increase was due to a temperature rise. Figure 2.32 compares the measured light intensity to the pressure rise for a mixture of  $\text{Br}_2$ ,  $\text{BrNO}$  and  $\text{NO}$  and to the expected intensity if the prompt pressure rise reflects a change in concentration in which the stoichiometry of the dark reaction is maintained. (The pressure and light intensity data shown in Figure 2.32 were recorded simultaneously using the lock-in amplifier and therefore are perfectly synchronized.) In this example, as in all of the runs with  $\text{BrNO}$  in the cell, the measured light intensity indicates that the prompt pressure increase is not due to a concentration change. The transmitted light intensity immediately after the prompt pressure rise agrees with the expected value calculated using the equilibrium concentrations of  $\text{Br}_2$  and  $\text{BrNO}$  and the value of  $I_0$  determined before the cell was filled, further confirming that the concentrations of  $\text{Br}_2$  and  $\text{BrNO}$  do not change during the prompt pressure rise. If the concentrations of  $\text{Br}_2$  and  $\text{BrNO}$  do not change the only reasonable explanation for the prompt jump is a rapid temperature rise immediately after the shutter opens. As in the  $\text{Br}_2$  cases, the temperature change after the shutter opens is

$$\Delta T = T_0 \left( \frac{P_{obs} - P_{calc}}{P_{calc}} \right) \quad (2.62)$$

$$= T_0 \left( \frac{\Delta P_{obs} - \Delta P_{calc}}{P_{calc}} \right) \quad (2.63)$$

The pressure rise in this example (about .3 torr) indicates that the temperature of the mixture increased by 1.5C in the second after the shutter opened. Since a temperature rise changes the equilibrium constant, upsetting the balance between the forward and reverse dark reactions, a temperature increase causes a concentration

change and, consequently, an additional pressure change, but this effect occurs slowly (Figures 2.33 and 2.34) and can be neglected during the prompt pressure jump.

The energy required to break the Br-N bond of BrNO is 1.206 eV (32), less than the 1.968 eV required to dissociate Br<sub>2</sub>, so more excess energy is available when BrNO is dissociated. However, the dissociation rate for BrNO is about a third that of Br<sub>2</sub> so the excess energy made available each second is less. The formation of Br\* when BrNO is dissociated is energetically possible at wavelengths less than 726 nm but any Br\* resulting from the dissociation of BrNO or Br<sub>2</sub> or would be rapidly quenched by inelastic collisions with Br<sub>2</sub>, NO or BrNO. The total rate constant for removal of Br\* by BrNO has been determined to be  $1.5 \pm 0.2 \times 10^{-11}$  cm<sup>3</sup>/molecule-s and the rate for quenching by NO is  $5.3 \times 10^{-12}$  cm<sup>3</sup>/molecule-s (59). Both NO and BrNO are therefore more efficient quenchers of Br\* than is Br<sub>2</sub>. Nearly all of the quenching occurs via inelastic collisions; indirect evidence suggests that the reaction  $\text{Br}^* + \text{BrNO} \rightarrow \text{Br}_2 + \text{NO}$  does not occur to a significant degree (59). The inelastic quenching collisions may yield vibrationally-excited Br<sub>2</sub>, NO or BrNO molecules. Wight (72) studied Br\* quenching by NO, finding that approximately 84% of the E→V collisions result in the formation of NO( $\nu = 2$ ) and 14% produce NO( $\nu = 1$ ) while production of the NO( $\nu = 0$ ) state is negligible. Sedlacek and Wight (59) found in later studies of Br\* quenching by BrNO that about 50% of the quenching collisions yield BrNO molecules excited in the  $\nu_1$  N-O bond stretching mode, with about six times as many in the  $\nu_1 = 1$  mode as in the  $\nu_1 = 2$  mode. Relaxation of the vibrationally-excited molecules occurs via V-V and V-T collisions. NO self-relaxation is dominated by V-V processes which are significantly faster than V-T relaxation of NO by NO (27).

In the bromine-only examples wall-recombination is the principle bromine atom recombination process. When BrNO is present the primary recombination mechanism is the reaction of bromine atoms with BrNO to form NO and Br<sub>2</sub>. The reaction is exothermic, releasing about .75 eV each time a ground state bromine atom reacts

with BrNO (48). The net result is to increase the temperature of the gas mixture. The bromine atoms produced by photodissociation of Br<sub>2</sub> and BrNO react rapidly with BrNO so the rate at which the gas is heated depends on the dissociation rates. Higher Br<sub>2</sub> and BrNO concentrations lead to larger dissociation rates and faster heating but also increase the heat capacity of the mixture. The NO contributes nothing to the heating but does contribute to the heat capacity of the mixture. Higher NO concentrations therefore reduce the temperature rise. These effects may be seen in Figures 2.35, 2.36 and 2.37, in which the temperature rise required to account for the initial pressure jump is plotted versus the equilibrium Br<sub>2</sub>, BrNO and NO pressures. In Figure 2.38 the temperature rise is plotted vs  $2 \times [\text{Br}_2]_{\text{eq}} + .33 \times [\text{BrNO}]_{\text{eq}}$ , which is approximately proportional to the number of Br atoms produced by photodissociation per second.

The heating effect occurs throughout the illuminated volume of the cell. The rapid temperature rise stops when heat loss to the walls of the cell balances the heat input from the dissociations. The temperature of the gas continues to rise slowly because the cell temperature increases and because the heat capacity of the gas decreases as BrNO is destroyed.

The precise reason the temperature rises has no bearing on the validity of the model for the later pressure rise. The transmitted light intensity provides a reliable determination of the Br<sub>2</sub> and BrNO concentrations and allows the temperature effects to be identified.

*2.7.5 Long-term Pressure Rise.* Figure 2.39 compares the pressure change calculated using Equation 2.61 to the data shown in Figure 2.27. The value of  $(\sigma_{\text{Br}_2} - 2 \sigma_{\text{BrNO}})$  that produces this fit is  $2.15 \times 10^{-19} \text{ cm}^2$  making  $\sigma_{\text{BrNO}}$  equal to  $2.08 \times 10^{-19} \text{ cm}^2$  for  $\sigma_{\text{Br}_2}$  equal to  $6.31 \times 10^{-19} \text{ cm}^2$ . These values are consistent with the values determined above. The pressures in steady state given by the fit are 3.6 torr Br<sub>2</sub>, 59.6 torr NO and .63 torr of BrNO. The pressure measured by the

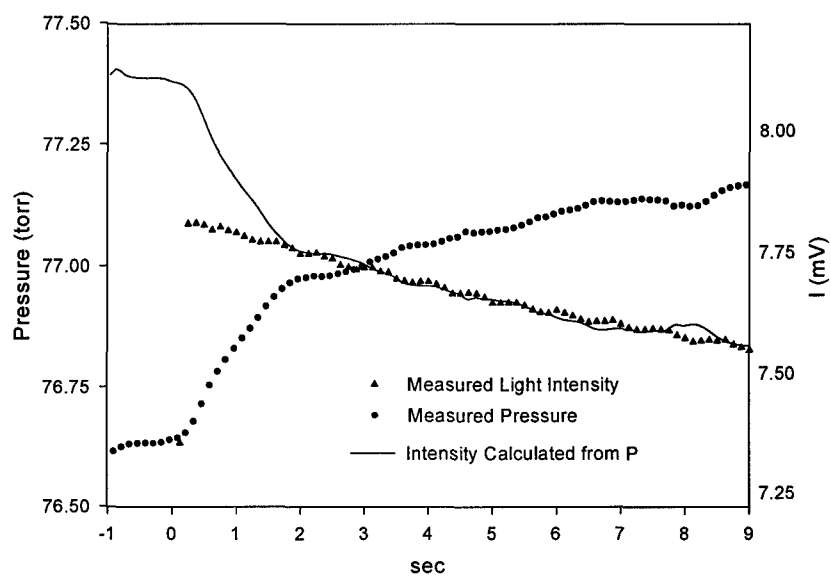


Figure 2.32 Comparison of prompt pressure change measured by manometer to measured light intensity and light intensity calculated assuming stoichiometry of dark reactions is maintained, for  $P_{NO}^{eq} = 40.5$  torr,  $P_{Br_2}^{eq} = 1.3$  torr and  $P_{BrNO}^{eq} = 21.5$  torr.

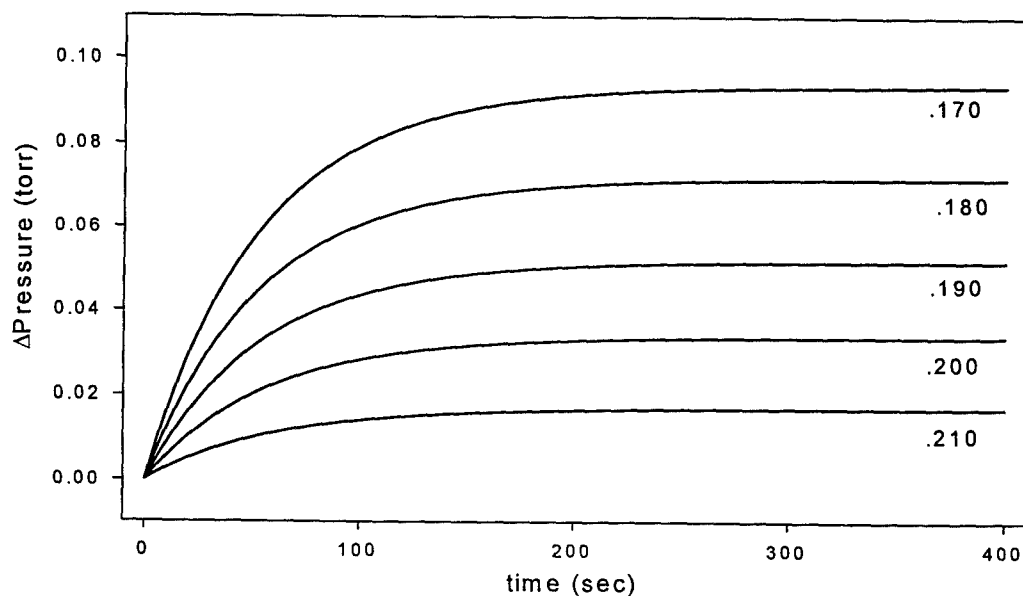


Figure 2.33 The slow concentration change resulting from an instantaneous temperature rise that changes  $K_{eq}$ , for a range of  $K_{eq}$  values. Calculated using the temperature dependence of  $K_{eq}$  reported by Houel (32) and of  $k_f$  reported by Hisatsune (31). The initial pressures are .403 torr  $\text{Br}_2$ , 9.194 torr  $\text{BrNO}$  and 30.806 torr  $\text{NO}$ . The temperature dependence of  $K_{eq}$  is shown in Figure 2.40.



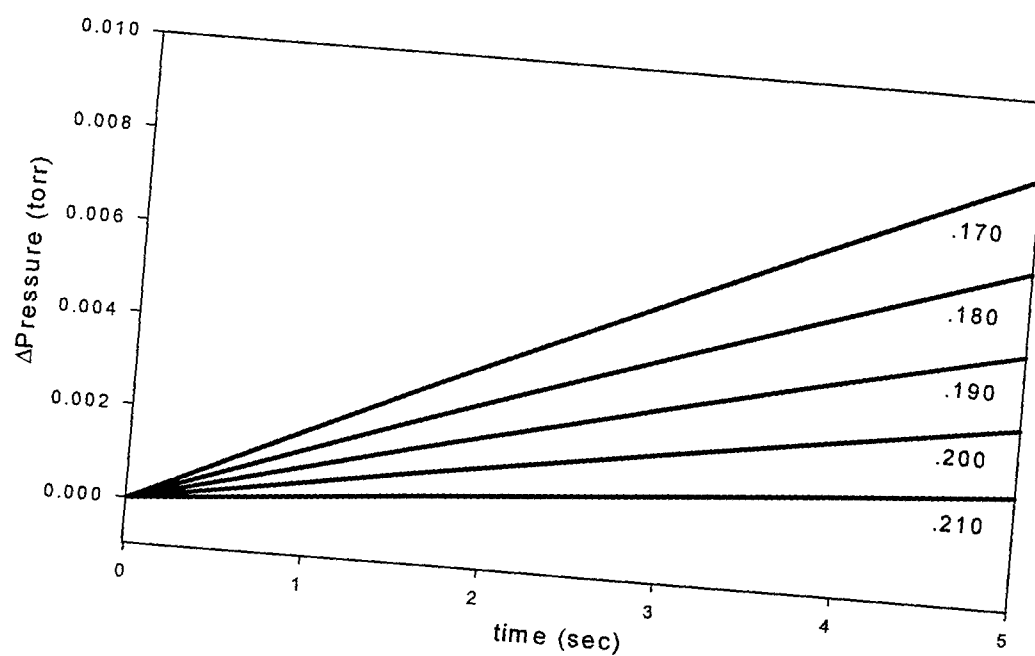


Figure 2.34 Same calculation as Figure 2.33, but shown for times less than 5 seconds.

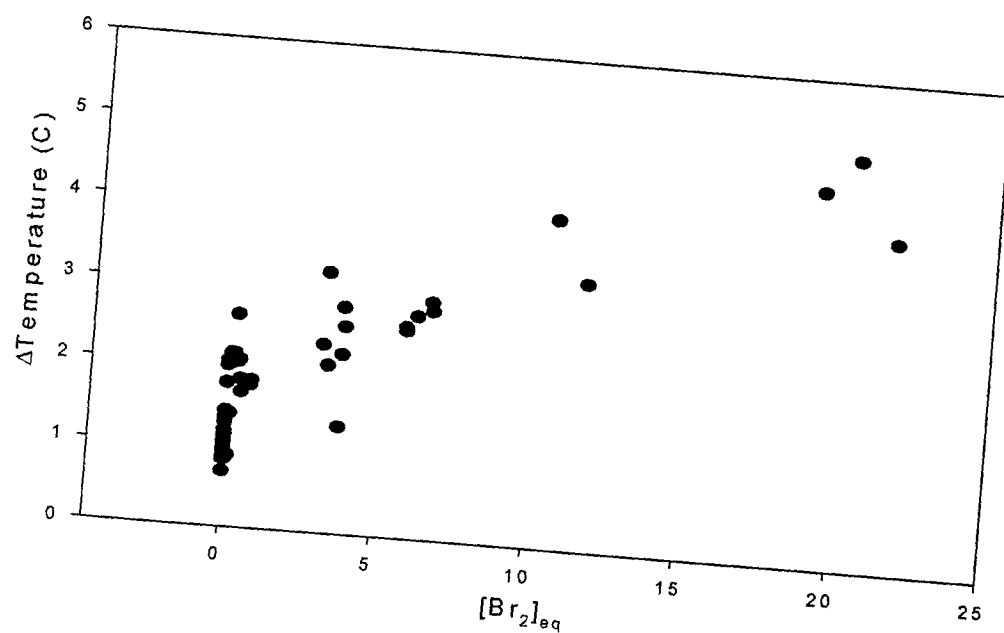


Figure 2.35 The magnitude of the prompt temperature rise increases as the equilibrium  $Br_2$  pressure rises.

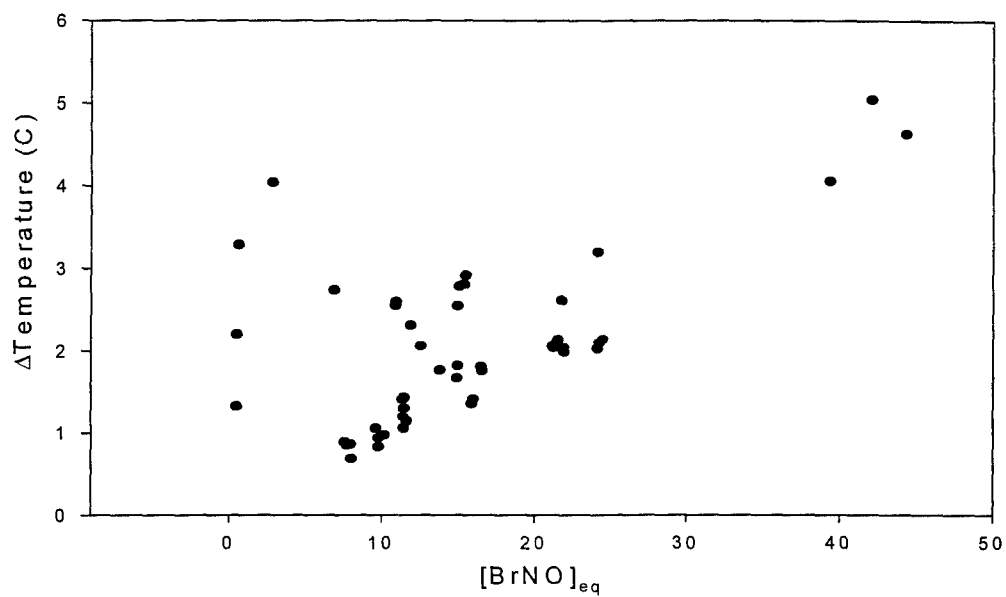


Figure 2.36 The magnitude of the prompt temperature rise tends to increase as the equilibrium  $\text{BrNO}$  pressure rises.

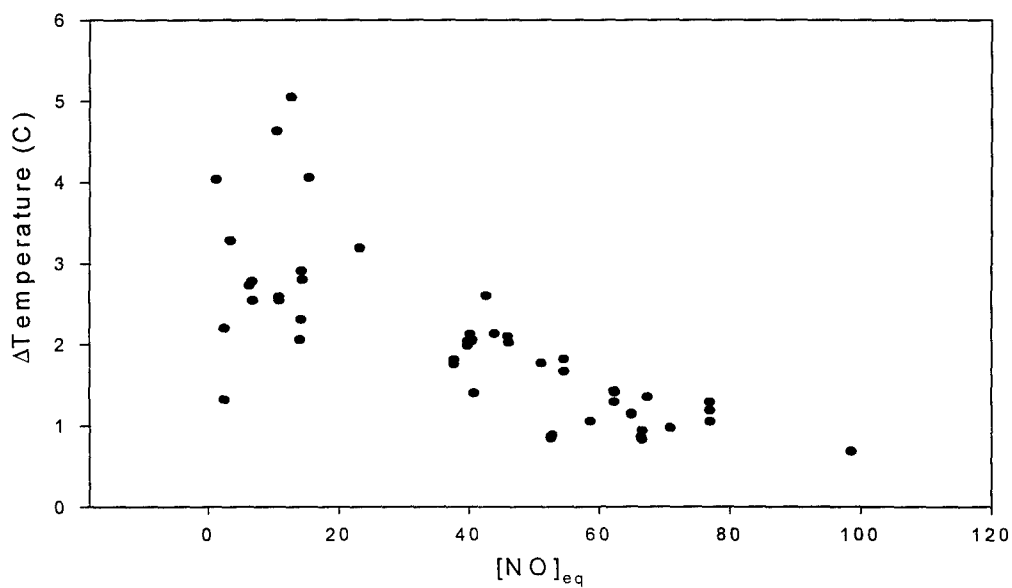


Figure 2.37 The magnitude of the prompt temperature rise decreases as the equilibrium  $\text{NO}$  pressure rises.

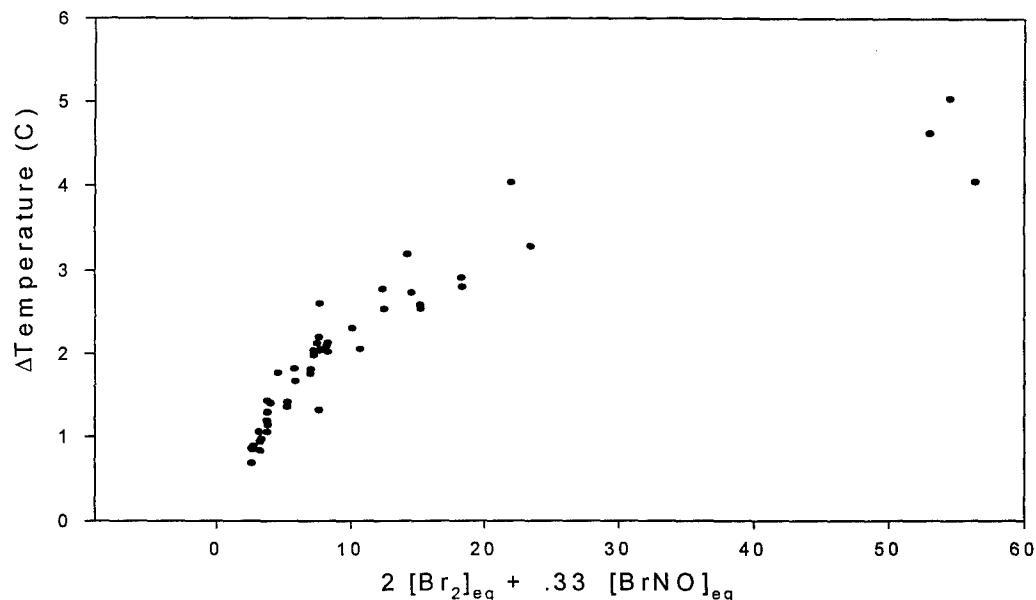


Figure 2.38 Prompt temperature rise when shutter opens vs.  $2 \times P_{\text{eq}}(\text{Br}_2) + .33 \times P_{\text{eq}}(\text{BrNO})$ .

manometer continues to increase after the calculated pressures of  $\text{Br}_2$ , NO and BrNO reach their steady state values. If the continuing pressure rise and the prompt jump are due entirely to increasing temperature, the gas is approximately 3C hotter when the shutter closes than it was when the shutter opened. The equilibrium constant change accounts for no more than .03 torr of the total pressure change of 3.75 torr.

The agreement of the calculated and measured concentrations after temperature effects are removed confirms only that the stoichiometry of the dark reaction is maintained. To confirm that the postulated set of equations adequately accounts for the pressure change the rate equations must be solved and the resulting time dependence of the total pressure or transmitted light intensity compared to the observed values.

When the bromine atom concentration is balanced by reaction with BrNO, the rate of change of the progress variable  $x(t)$  derived from Equations 2.58, 2.59 or 2.60

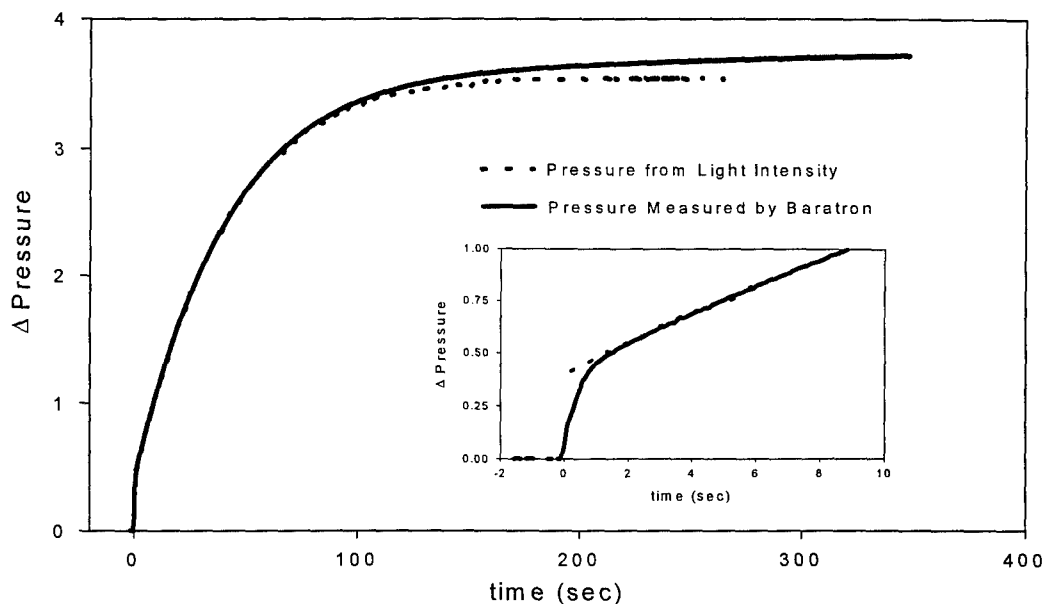


Figure 2.39 Pressure change calculated from transmitted light intensity compared to that measured by manometer.

is

$$\begin{aligned} \frac{dx}{dt} = & k_p^{Br_2} I_p ([Br_2]_0 + x) + k_p^{BrNO} I_p ([BrNO] - 2x) \\ & - k_f([Br_2]_0 + x)([NO]_0 + 2x)^2 + k_r([BrNO]_0 - 2x)^2 \end{aligned} \quad (2.64)$$

which can be integrated as in Section 2.5.1 and fit to the data. The additional terms in Equation 2.64, however, do not allow so simple a fitting process. One way around this problem is to use the final pressure and the slope of the pressure change at  $t = 0$  to derive two equations that can be solved simultaneously for the rate constants. If the initial pressures are the equilibrium pressures just before the shutter opens and  $x_f$  is the total pressure change corrected for temperature effects, the equations are:

$$\begin{aligned} \frac{dx}{dt}(t = 0) = & k_p^{Br_2} I_p [Br_2]_{eq} + k_p^{BrNO} I_p [BrNO]_{eq} \\ & - k_f[Br_2]_{eq} [NO]_{eq}^2 + k_r[BrNO]_{eq}^2 \end{aligned} \quad (2.65)$$

$$\begin{aligned}
0 = & k_p^{Br_2} I_p ([Br_2]_{eq} + x_f) + k_p^{BrNO} I_p ([BrNO]_{eq} - 2 x_f) \\
& - k_f ([Br_2]_{eq} + x_f) ([NO]_{eq} + 2x_f)^2 \\
& + k_r ([BrNO]_{eq} - 2 x_f)^2
\end{aligned} \tag{2.66}$$

The value of the equilibrium constant determined in section 2.5 allows one of the rate constants to be eliminated from the equations; a reasonable assumption that eliminates one of the dissociation rates is that the ratio of the  $Br_2$  and  $BrNO$  dissociation rates equals the ratio of  $\alpha_{Br_2}$  and  $\alpha_{BrNO}$ . Although a simultaneous solution to these two equations will always match the endpoints of the pressure trace, it is unlikely to replicate the rest of the data unless the model is correct.

The temperature rise responsible for the prompt pressure jump after the shutter opens lowers the dark reaction equilibrium constant. This disturbs the dark reaction equilibrium and makes a positive contribution to the initial slope. As the temperature of the mixture continues to increase during the long-term pressure rise the effect on the equilibrium constant becomes more pronounced, but any concentration changes caused by the temperature rise will be seen in the transmitted light intensity. The prompt pressure jump can be used to estimate the temperature of the gases in the cell at the beginning of the long-term pressure rise and the equilibrium constant varied accordingly.

The variation of  $k_f$  and  $k_r$  with temperature may be estimated using the reported temperature dependence of  $K_{eq}$  and  $k_f$ :

$$\begin{aligned}
\ln K_{eq}(T) &= \ln K_{eq}(293) + \frac{\Delta H^0}{R} \left( \frac{1}{293} - \frac{1}{T} \right) \\
\ln k_f(T) &= \ln k_f(293) + \frac{E_{act}}{R} \left( \frac{1}{293} - \frac{1}{T} \right) \\
\ln k_r(T) &= \ln k_f(T) - \ln K_{eq}(T)
\end{aligned}$$

Houel (32) measured the equilibrium constant over the temperature range 263- 333K, finding that  $\Delta H^0$  is  $-10.71 \pm 1.86$  kcal/mol. Figure 2.40 shows the variation of  $K_{eq}$

with temperature using this result. Houel determined that the apparent activation energy for the forward reaction is  $1.35 \pm 1.27$  kcal/mol. Hisatsune (31) reported a value over the temperature range 263-333K of  $0.573 \pm 0.30$  kcal/mol and Krauss (39) a value of  $1.5 \pm 1$  kcal/mol over the temperature range 265- 288K. Figure 2.41 shows the variation of  $k_f$  predicted by Houel's results and Figure 2.42 is the variation of  $k_r$  calculated from the variation of  $K_{eq}$  and  $k_f$ . In these plots the values of  $K_{eq}$ ,  $k_f$  and  $k_r$  at 293K were taken as the values determined in the current experiment, not those determined by Houel, and the dashed lines show the range of variation allowed by the errors in  $\Delta H^0$  and  $E_{act}$ .

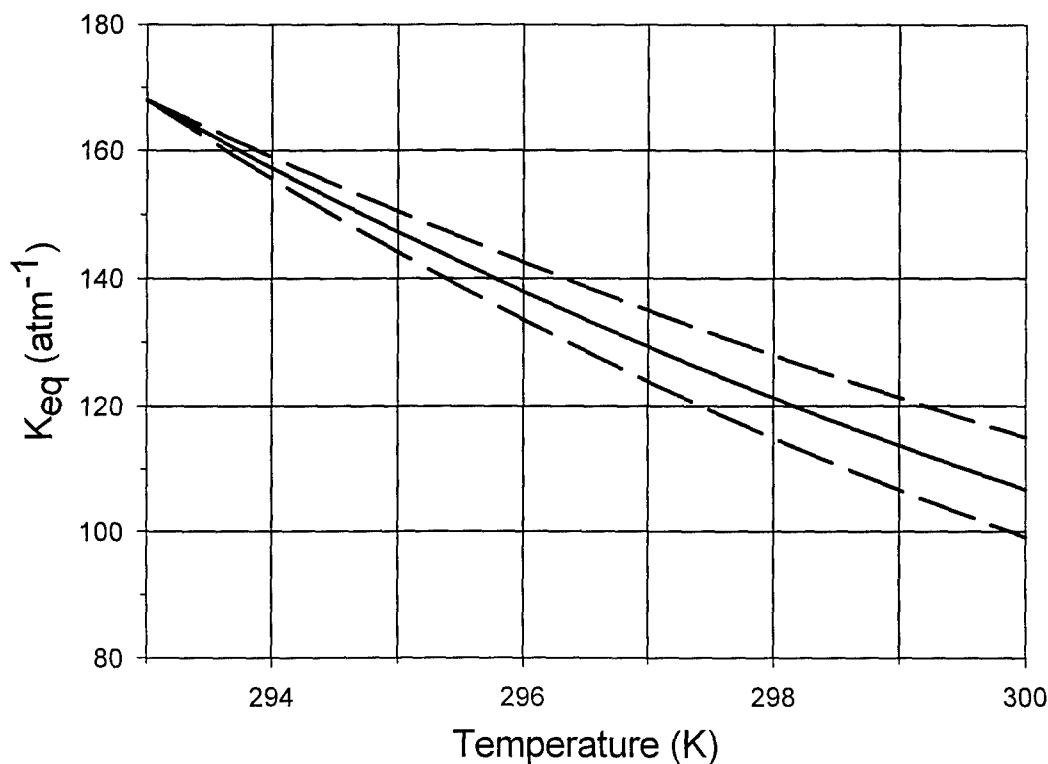


Figure 2.40 Variation with temperature of  $K_{eq}$ , calculated using  $\Delta H^0 = -10.71 \pm 1.86$  kcal/mol (32).

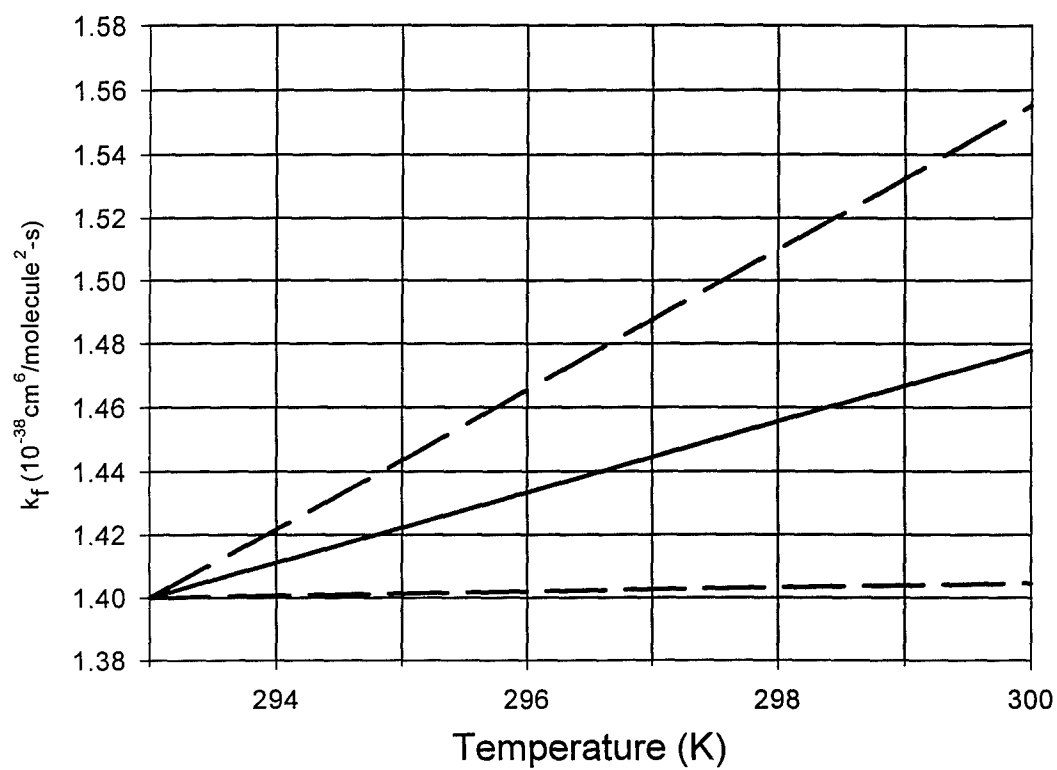


Figure 2.41 Variation with temperature of  $k_f$ , calculated using  $E_{act} = 1.35 \pm 1.27$  cal/mol (32).

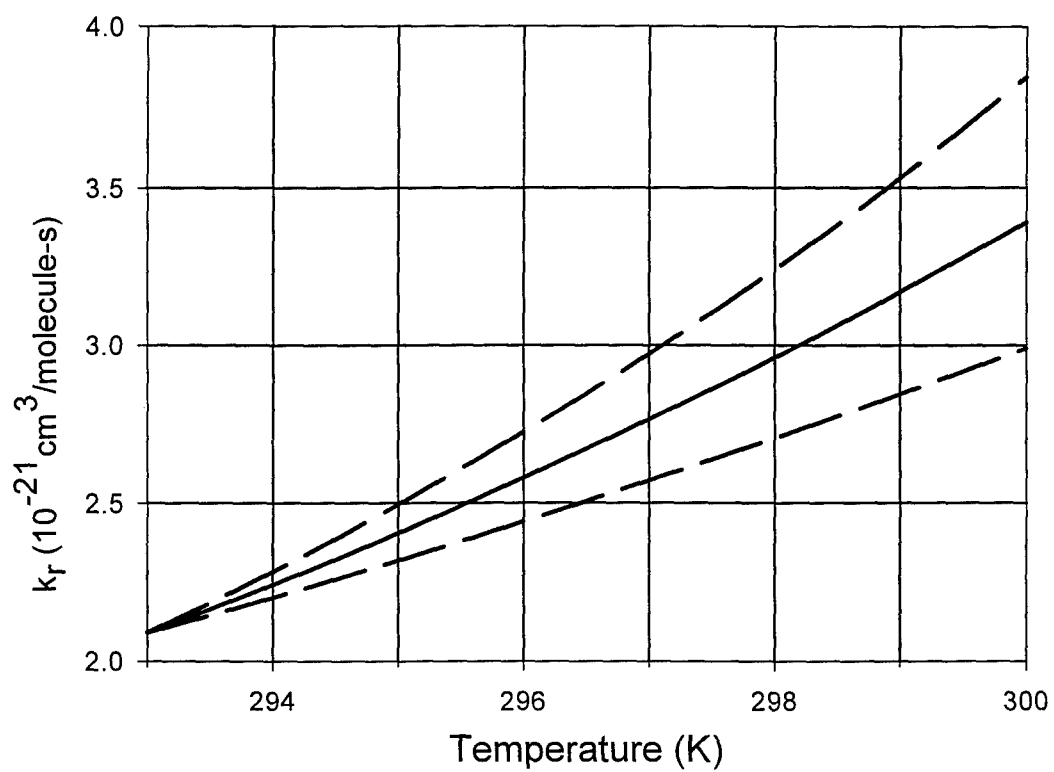


Figure 2.42 Variation with temperature of  $k_r$ , calculated using temperature dependencies of  $K_{eq}$  and  $k_f$  reported by Houel (32)



In these experiments the initial BrNO concentration is always nonzero. In some cases all of the BrNO initially present is converted into Br<sub>2</sub> and NO and the Br concentration is controlled by wall and three-body recombination. In steady state the reactions that include BrNO can be ignored but to model the concentration changes from the time the shutter opens until steady-state is reached the full set of reactions must be solved numerically.

*2.7.6 Examples and Discussion.* Equation 2.66 predicts that  $x_f$  is very small when the initial NO concentration is large and the initial bromine concentration is almost zero. Very little of the BrNO is converted into Br<sub>2</sub> under these conditions. Figure 2.43 shows the transmitted light intensity for a mixture containing almost no Br<sub>2</sub>. In this case about 150 torr of NO was added to 7.5 torr of bromine, making the equilibrium pressures before the shutter opened approximately .05 torr Br<sub>2</sub>, 14.9 torr BrNO and 135.1 torr NO. The light intensity indicates that the Br<sub>2</sub> concentration changed by no more than .01 torr after the shutter opened. (This data was obtained using the cell with Pyrex windows.) The transmitted intensity when the cell was empty was 17.5 mV, which makes  $\alpha_{\text{BrNO}} = .123 \text{ torr}^{-1}$  for  $\alpha_{\text{Br}_2} = .373 \text{ torr}^{-1}$ . Ignoring the small Br<sub>2</sub> concentration leads to a 1.1% error in the value of  $\alpha_{\text{BrNO}}$ .)

Figures 2.44, 2.45, 2.46 and 2.47 are examples of runs made using the 20 cm cell with CaF<sub>2</sub> windows. In each of these figures the pressure change calculated from the light intensity is compared to the model prediction. The model gives an excellent fit to the data. The initial pressures and the results of the fits are listed in Table 2.6. The fit shown in Figure 2.44 is not as good as that shown in the other figures; in this case the calculated pressure drops after the photo-stationary state is reached, indicating that bromine is disappearing. This affects not only the final pressure but also the shape of the pressure versus time curve and is not incorporated into the model. Adjusting the initial pressures would improve the fit.

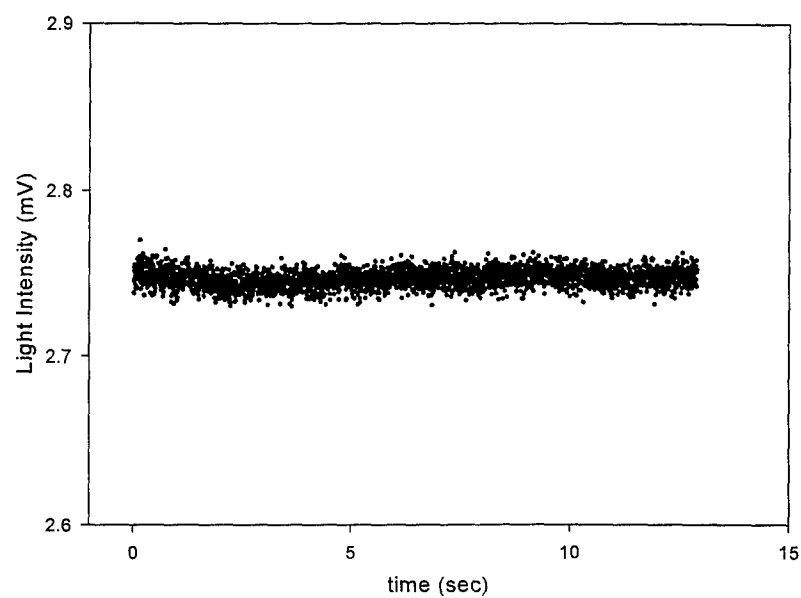


Figure 2.43 The transmitted light intensity for 150 torr of NO added to 7.5 torr  $\text{Br}_2$ .

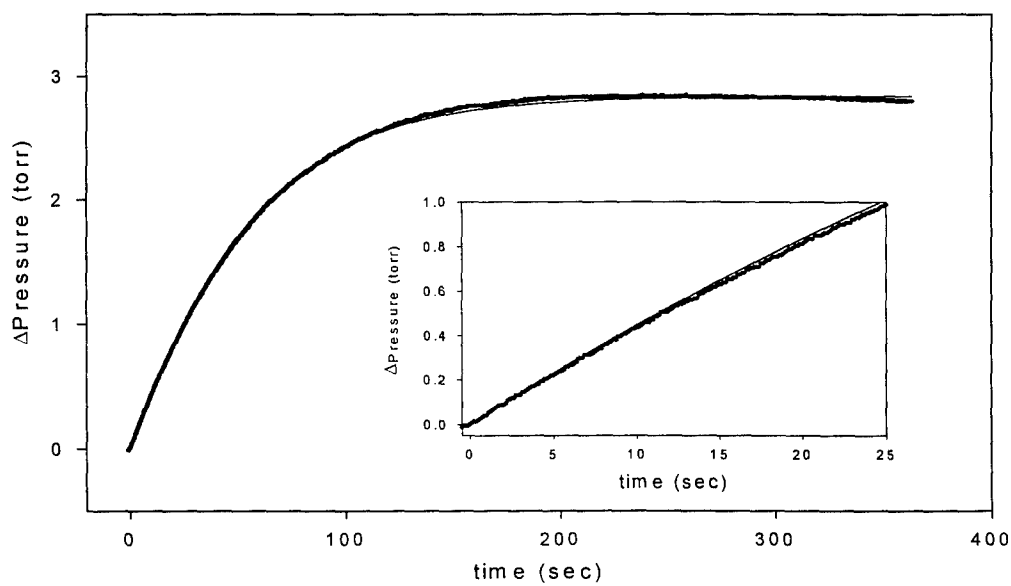


Figure 2.44 Comparison of pressure rise calculated from the light intensity to that predicted by the model. See Table 2.6 for initial pressures and results of fit.

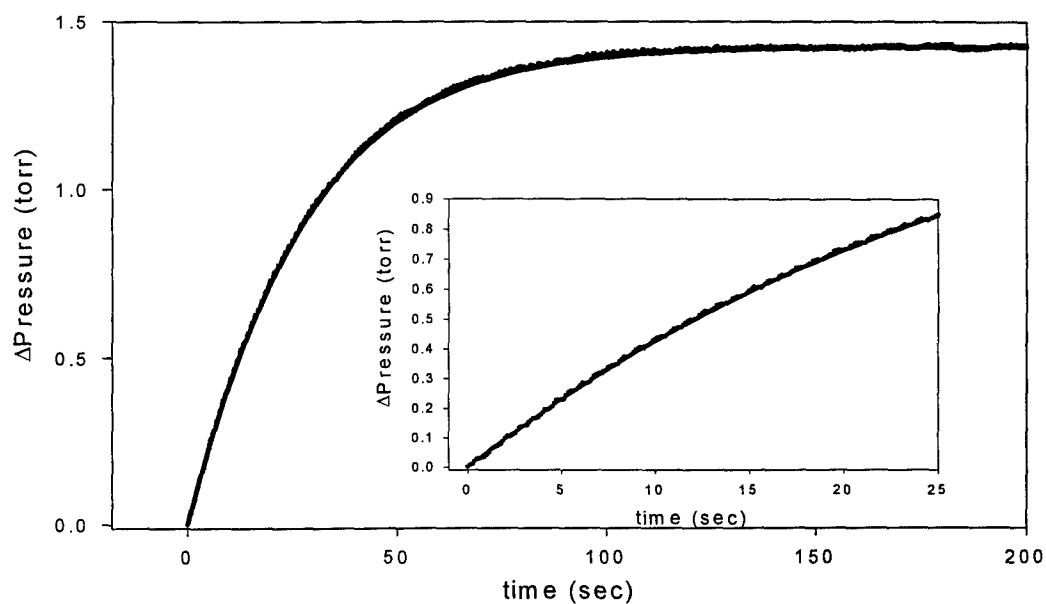


Figure 2.45 Comparison of pressure rise calculated from the light intensity to that predicted by the model. See Table 2.6 for initial pressures and results of fit.

Table 2.6 Initial pressures and constants derived from fits, using 20 cm long cell. The temperature of the gas mixture before the prompt temperature rise was taken as 293K.

Figure	2.44	2.45	2.46	2.47
$P(\text{Br}_2)_{\text{eq}}$ (torr)	3.08	.78	.13	$\approx 0$
$P(\text{BrNO})_{\text{eq}}$ (torr)	11.9	16.50	7.56	$\approx 8$
$P(\text{NO})_{\text{eq}}$ (torr)	14.2	37.72	52.7	$\approx 99$
$\Delta T_i$ (K)	2.34	1.81	1.04	0.8
slope (torr/s)	.046	.049	.025	.021
$P(x_f)$ (torr)	2.83	1.43	1.42	.17
$k_f$ ( $10^{-38}$ cm <sup>6</sup> /molecule <sup>2</sup> -s)	2.29	1.66	1.58	1.17
$k_r$ ( $10^{-21}$ cm <sup>3</sup> /molecule-s)	3.42	2.79	2.36	1.74
$k_p^{Br_2} I_p$ (s <sup>-1</sup> )	.006	.007	.011	.007

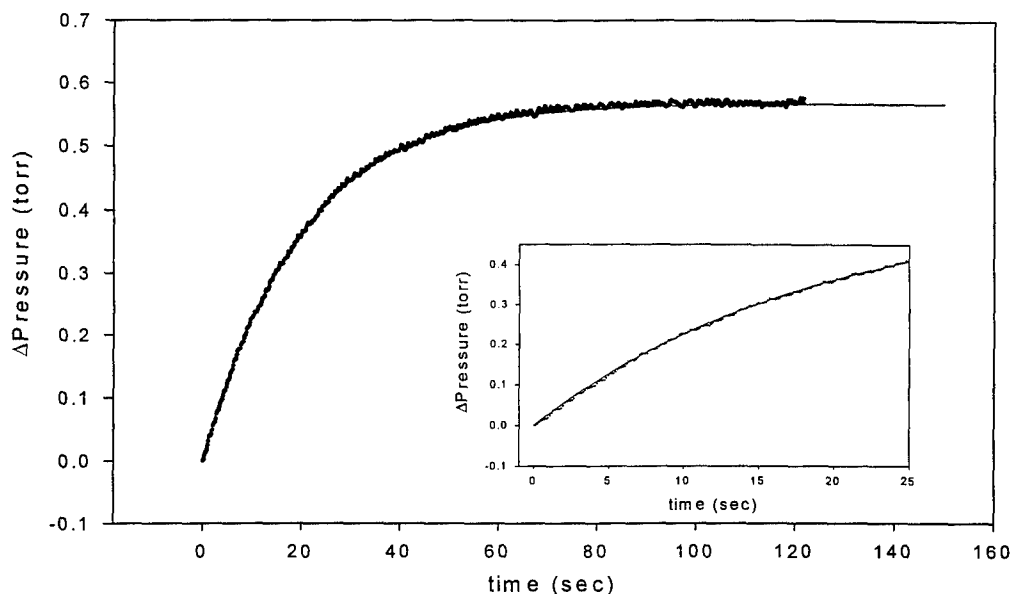


Figure 2.46 Comparison of pressure rise calculated from the light intensity to that predicted by the model. See Table 2.6 for initial pressures and results of fit.

Figures 2.48, 2.50, 2.52 and 2.54 are examples of runs using the 18 cm long cell with Pyrex windows. The initial pressures and fit results for each figure are listed in Table 2.7. The value of  $\sigma_{\text{Br}_2} - 2\sigma_{\text{BrNO}}$  that scales the calculated pressure rises correctly is  $2.126 \times 10^{-19} \text{ cm}^2$ , or almost exactly the value determined when the longer cell is used. The temperature changes for these examples, calculated using Equation 2.63 with  $T_0 = 293\text{K}$ , are shown in Figures 2.49, 2.51, 2.53 and 2.55. These plots show the rapid initial rise followed by a slower, approximately linear rise that characterizes these runs.

Figures 2.56 and 2.57 plot the forward and reverse rates determined from the fits against the temperature rise  $\Delta T_i$  determined from the prompt pressure rise. The rates increase with temperature, as expected, but somewhat faster than the predictions made estimated using the published values of  $E_{\text{act}}$  and  $\Delta H^0$  (Figures 2.41 and 2.42).

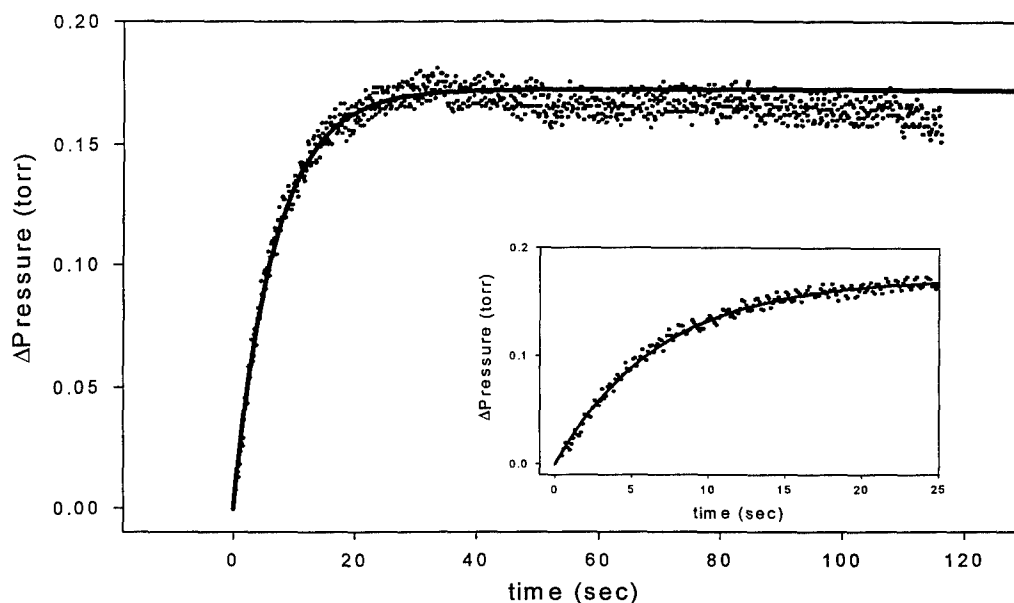


Figure 2.47 Comparison of pressure rise calculated from the light intensity to that predicted by the model. See Table 2.6 for initial pressures and results of fit.

Table 2.7 Initial pressures and constants derived from fits, using 18 cm long cell. The temperature of the gas mixture before the prompt temperature rise was taken as 293K.

Figure	2.48	2.50	2.52	2.54
$P(\text{Br}_2)_{\text{eq}}$ (torr)	4.16	.82	.27	.1
$P(\text{BrNO})_{\text{eq}}$ (torr)	9.48	20.77	11.59	8.81
$P(\text{NO})_{\text{eq}}$ (torr)	9.89	48.83	47.09	60.37
$\Delta T_i$ (K)	1.60	1.76	1.10	.70
slope (torr/s)	.027	.051	.036	.043
$P(x_f)$ (torr)	2.70	1.10	.86	.40
$k_f$ ( $10^{-38} \text{ cm}^6/\text{molecule}^2\text{-s}$ )	1.95	1.43	1.34	1.28
$k_r$ ( $10^{-21} \text{ cm}^3/\text{molecule-s}$ )	3.05	2.24	2.00	1.91
$k_p^{Br_2} I_p$ ( $\text{s}^{-1}$ )	.004	.006	.008	.007

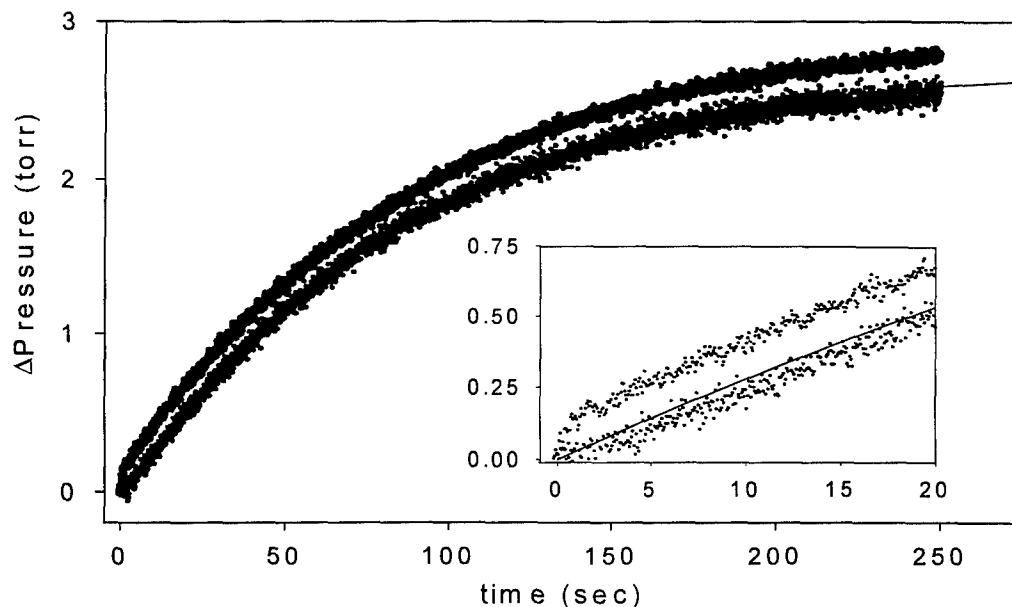


Figure 2.48 Comparison of pressure rises calculated from the light intensity, measured by manometer, and predicted by model. See Table 2.7 for initial pressures and results of fit.

The reason the  $k_p^{Br_2} I_p$  values determined from these fits are consistently smaller than the value determined in the bromine-only experiments, about  $.050 \text{ s}^{-1}$ , is not clear. There is no evidence that the concentrations change quickly after the shutter opens; if the concentrations do not change the dark reactions are still approximately balanced for the first few seconds after the shutter opens and contribute very little to the initial slope of the long-term pressure rise. The initial slope is therefore a direct measurement of the photolysis rates. Including the effect of temperature on the equilibrium constant makes the value of  $k_p^{Br_2} I_p$  determined from the fits even smaller because a temperature rise increases  $k_r$  relative to  $k_f$ , making a positive contribution to the initial slope. For temperature rises of a few degrees C, however, this effect is negligible. Although the light intensity varied somewhat during the course of these experiments as the apparatus configuration changed, the bromine-only results were often obtained just before the NO was added to the bromine. The

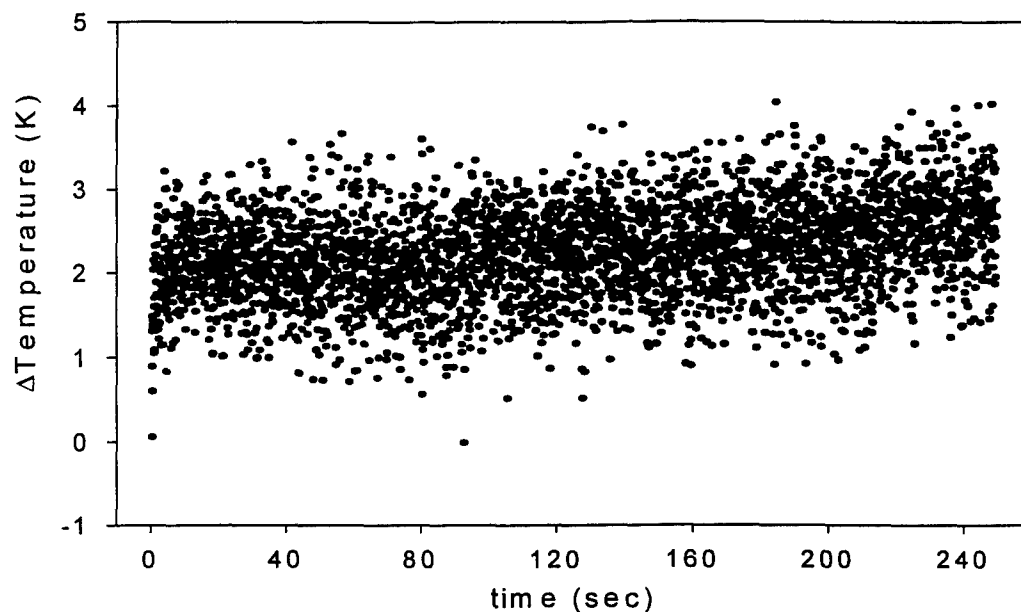


Figure 2.49 The temperature rise for the data of Figure 2.48, calculated from the difference between the pressure rise measured by the manometer and the rise calculated using the transmitted light intensity.

$k_p I_p$  values are averages over the length of the cell and the bromine-only results show that they decrease as the concentration of the absorbing species increases. The sum of the bromine and BrNO concentrations in the mixtures was never as high as the bromine concentration was in some of the bromine-only cases; since the BrNO absorption coefficient is less than that of Br<sub>2</sub> for wavelengths larger than about 375 nm this effect would be more pronounced for the mixtures only if the light at wavelengths below 375 nm drive the reactions. Experiments with short-pass filters, however, showed that the wavelengths below 450 nm contribute very little to the pressure rise seen in the mixtures (Figure 2.30).

Figure 2.58 demonstrates that the initial slope is primarily a function of the photolysis rate, which is approximately proportional to the light intensity. The figure compares two successive runs, one with a neutral density filter placed between the lamp and the cell and one without the filter. The value of  $k_p^{Br_2} I_p$  determined from

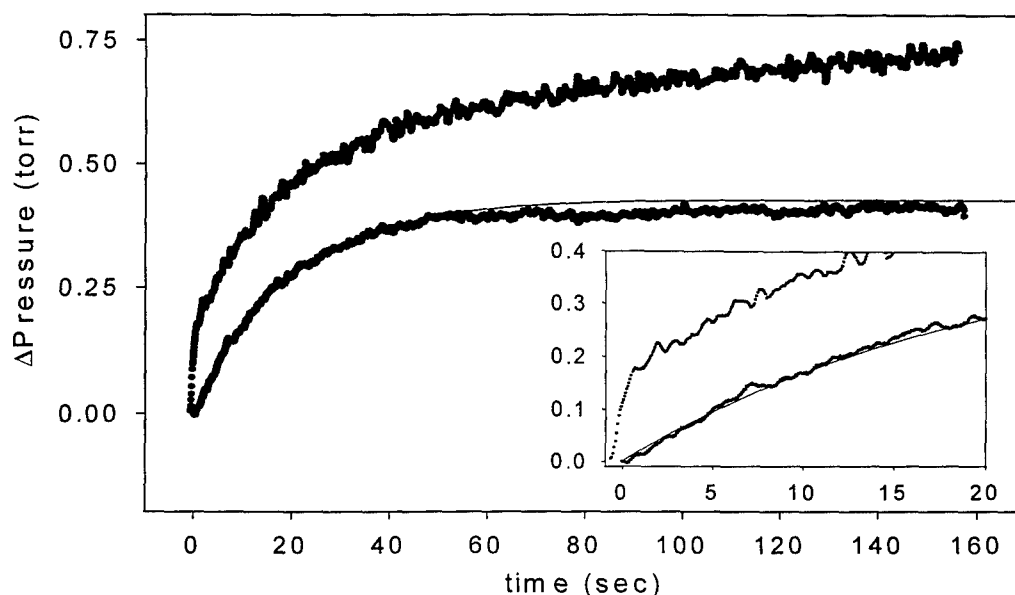


Figure 2.50 Comparison of pressure rises calculated from the light intensity, measured by manometer, and predicted by model. See Table 2.7 for initial pressures and results of fit.

the fit to the data from the run without a filter is  $.0072 \text{ s}^{-1}$ , four times larger than  $.0018 \text{ s}^{-1}$ , the value for the run with the ND filter. The ratio of the transmitted light intensity immediately after the shutter opened for the two cases is 4.9, somewhat higher than the ratio of the two values of  $k_p^{Br_2} I_p$ .

The  $k_p^{Br_2} I_p$  values determined from the mixture fits could be lower because the model omits a reaction that removes  $Br_2$  from the system. The excellent agreement between the predictions of the model, the concentration changes determined from the transmitted light intensity data, and the observed pressure change (when temperature affects are accounted for) suggests that the model does not omit any significant reaction. To be important, any omitted reaction that depends on the presence of Br atoms would have to be about as fast as the reaction between Br atoms and BrNO molecules and would have to produce something other than BrNO and NO. There is no evidence from the light intensity that anything other than  $Br_2$ , BrNO and NO



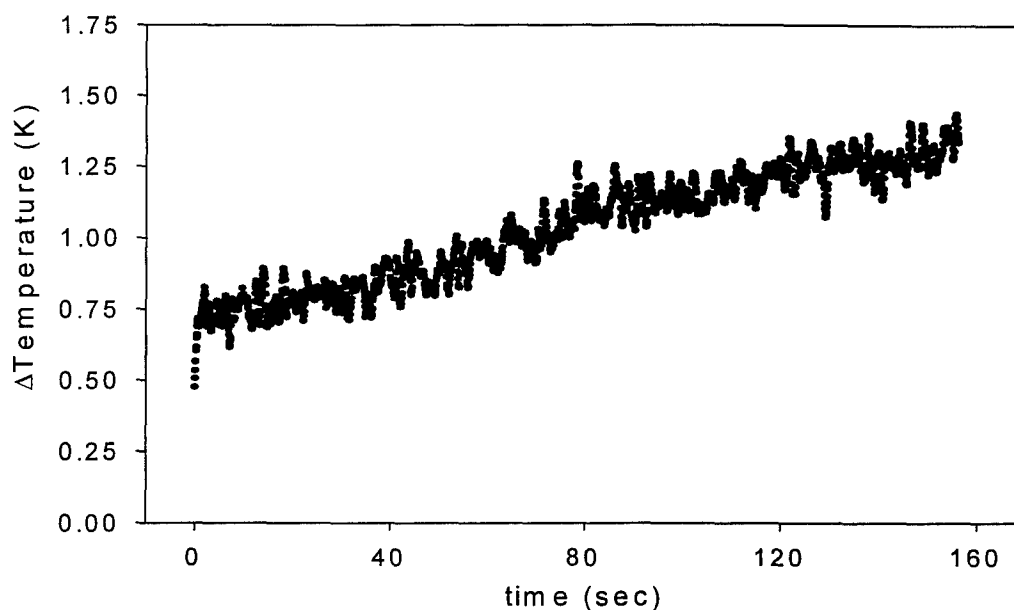


Figure 2.51 The temperature rise for the data of Figure 2.50, calculated from the difference between the pressure rise measured by the manometer and the rise calculated using the transmitted light intensity.

is in the cell after the shutter opens. If an overlooked reaction does not depend on the Br concentration it would be expected to influence the dark reaction results, but there is no evidence from the dark reaction experiments that suggests such an effect.

In summary, the model matches the data over the range of conditions where it is expected to work and produces consistent, reproducible values for the rate constants. The lower  $k_p$   $I_p$  values are almost certainly correct, but the reason they are lower is not fully understood.

This simple model predicts that the BrNO concentration after the photo-stationary state is reached is smaller for lower initial NO pressures. When the BrNO concentration becomes negligible the simple model fails and the full set of reactions must be solved numerically to accurately model the pressure change. Figure 2.59 shows what happens when 4.0 torr of NO is added to 11.9 torr of Br<sub>2</sub>. When the shutter was opened (before the mixture reached equilibrium) the cell contained .59

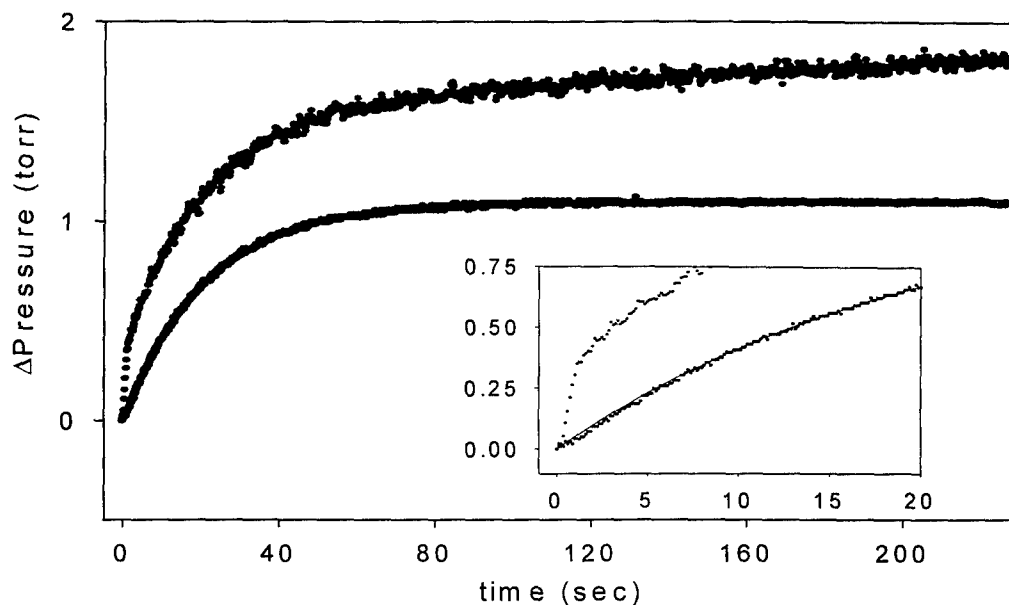


Figure 2.52 Comparison of pressure rises calculated from the light intensity, measured by manometer, and predicted by model. See Table 2.7 for initial pressures and results of fit.

torr BrNO, 11.6 torr Br<sub>2</sub> and 3.4 torr NO. The steady-state pressure with the shutter open, 16.06 torr, is .16 torr higher than the sum of the initial NO and Br<sub>2</sub> pressures. If this pressure excess reflects the bromine atom concentration about 1.4% of the molecular bromine originally present has been dissociated, consistent with the earlier bromine-only examples. The gradual pressure drop after the photostationary state is reached is due to bromine loss to the walls of the apparatus.

*2.7.7 Summary.* When an equilibrium mixture of Br<sub>2</sub>, NO and BrNO is disturbed by photolysis, BrNO is rapidly removed by reaction with atomic bromine. For continuous photolysis, a new photostationary condition is achieved which shifts the equilibrium toward Br<sub>2</sub> and NO. If the new BrNO concentration is not zero the steady-state Br concentration will be very small; the bromine atoms liberated by photodissociation of Br<sub>2</sub> and BrNO are immediately converted into Br<sub>2</sub> and NO by

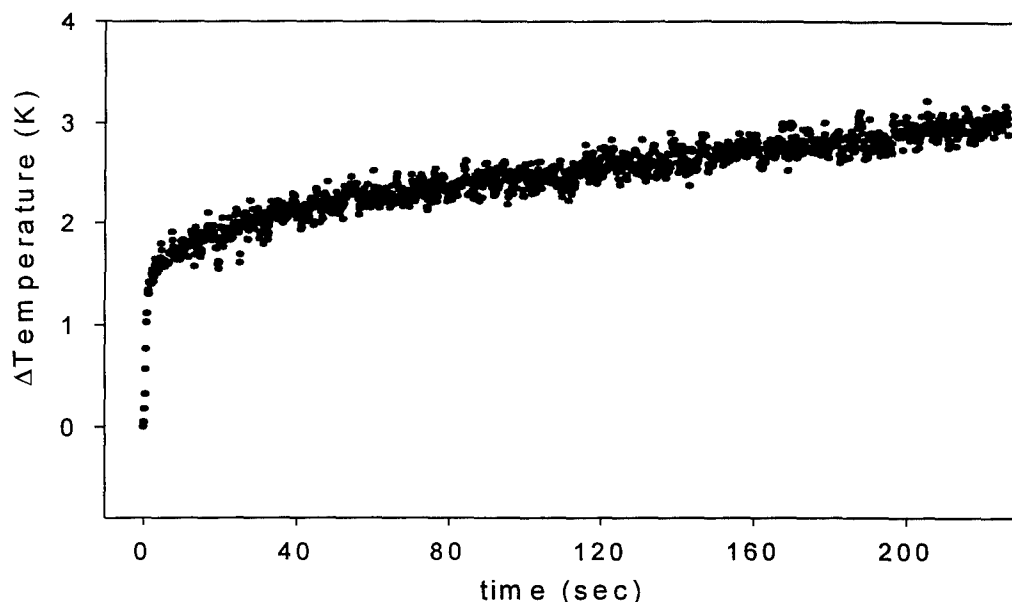
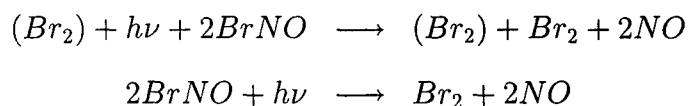


Figure 2.53 The temperature rise for the data of Figure 2.52, calculated from the difference between the pressure rise measured by the manometer and the rise calculated using the transmitted light intensity.

a kinetic mechanism equivalent to:



The photolysis of  $Br_2$  in conjunction with the reaction of Br atoms with BrNO gives a net gain of one bromine molecule and two NO molecules for each bromine molecule dissociated. The simultaneous photolysis of BrNO results in the destruction of BrNO with a quantum yield of 2.

This kinetic mechanism and rates for the photolysis of mixtures of  $Br_2$ , NO and BrNO has been validated for total pressures of 28-111 torr and nitric oxide to molecular bromine concentration ratios of 2.18-26.75, with an average  $Br_2$  photolysis rate of 0.050 molecules/s.

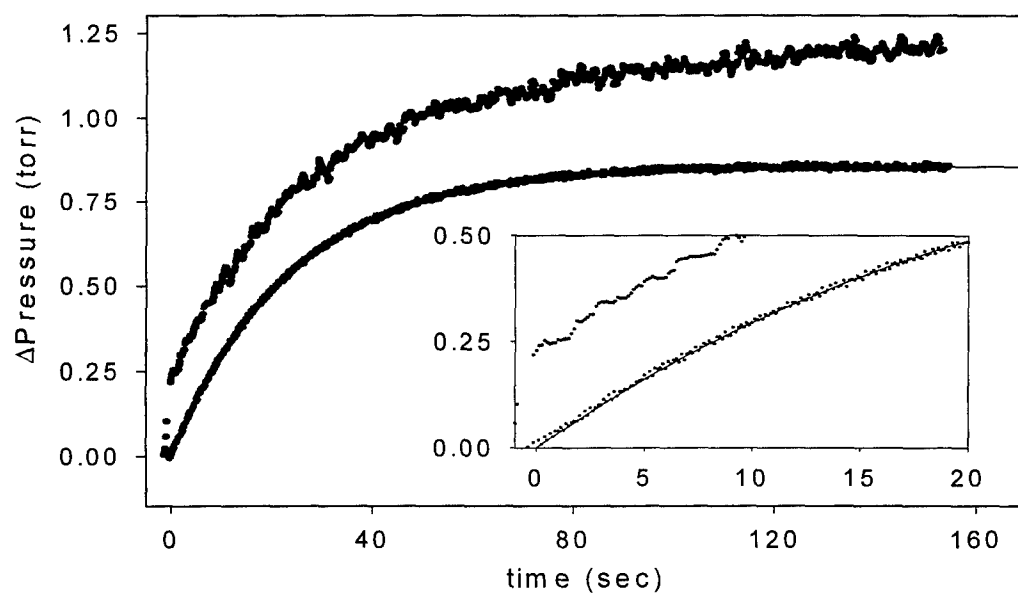


Figure 2.54 Comparison of pressure rises calculated from the light intensity, measured by manometer, predicted by model. See Table 2.7 for initial pressures and results of fit.

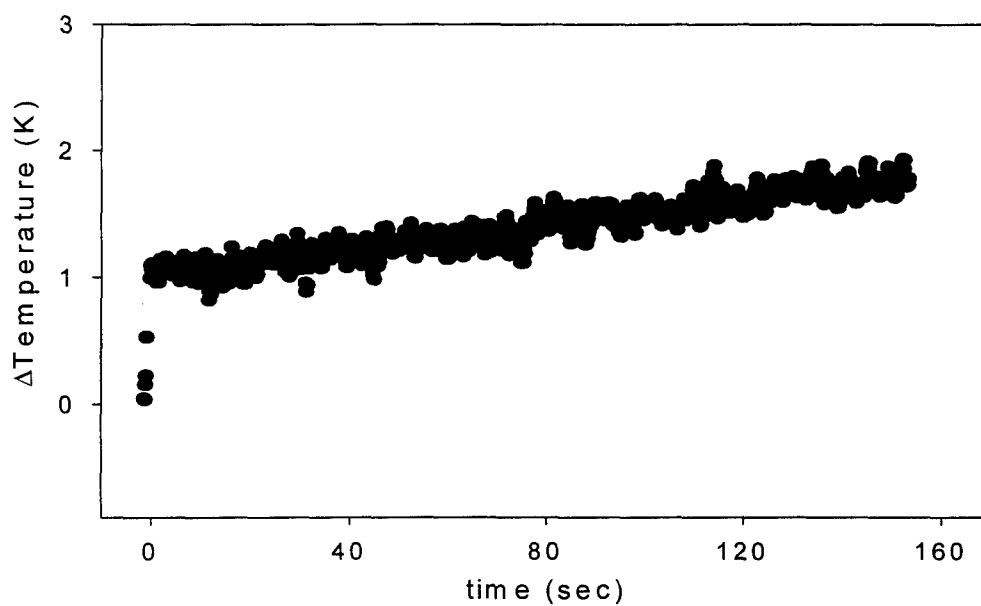


Figure 2.55 The temperature rise for the data of Figure 2.54, calculated from the difference between the pressure rise measured by the manometer and the rise calculated using the transmitted light intensity.

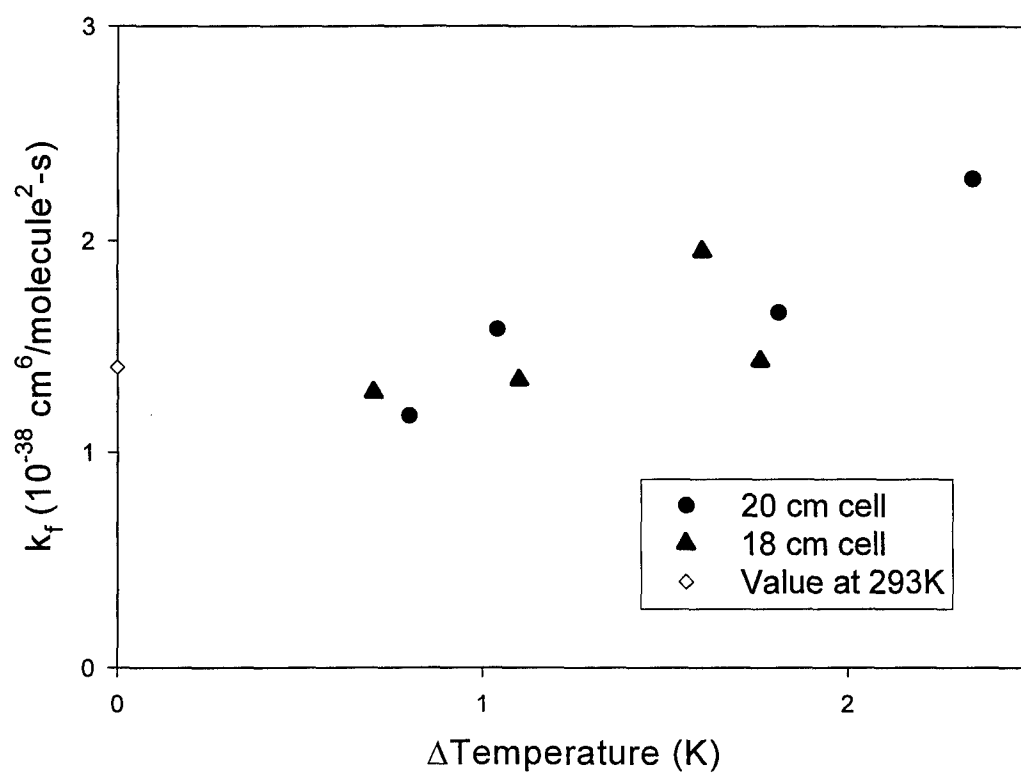


Figure 2.56 Comparison of forward rate constant  $k_f$  determined from fits to temperature rise determined from initial prompt pressure jump.

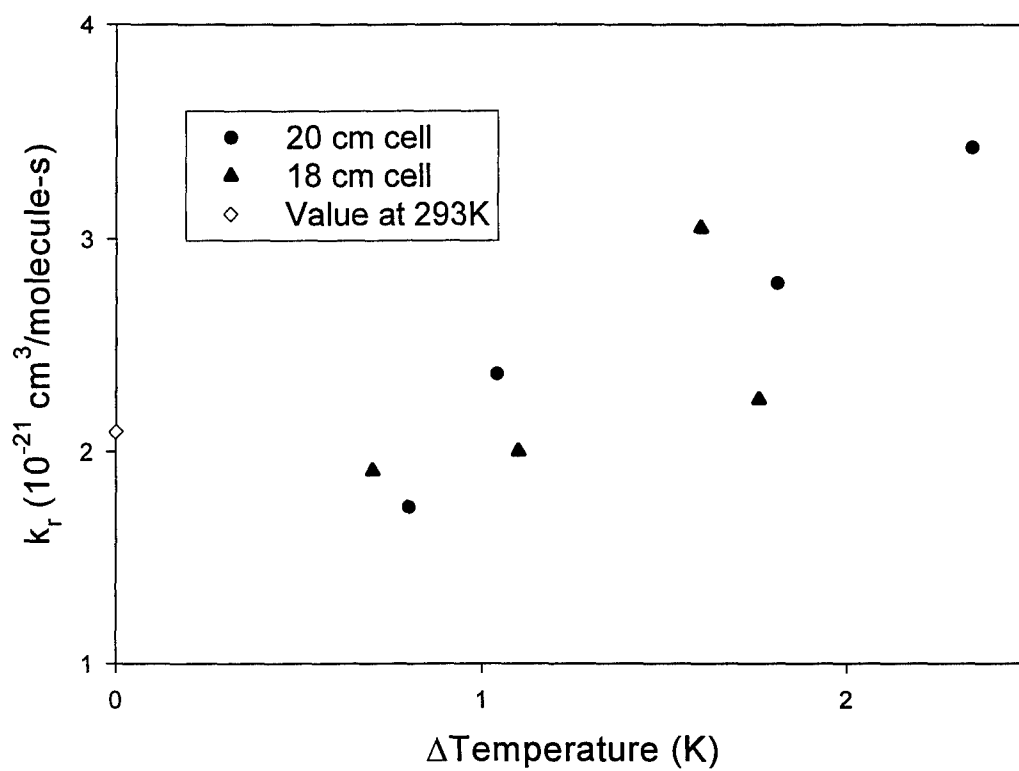


Figure 2.57 Comparison of reverse rate constant  $k_r$  determined from fits to temperature rise determined from initial prompt pressure jump.

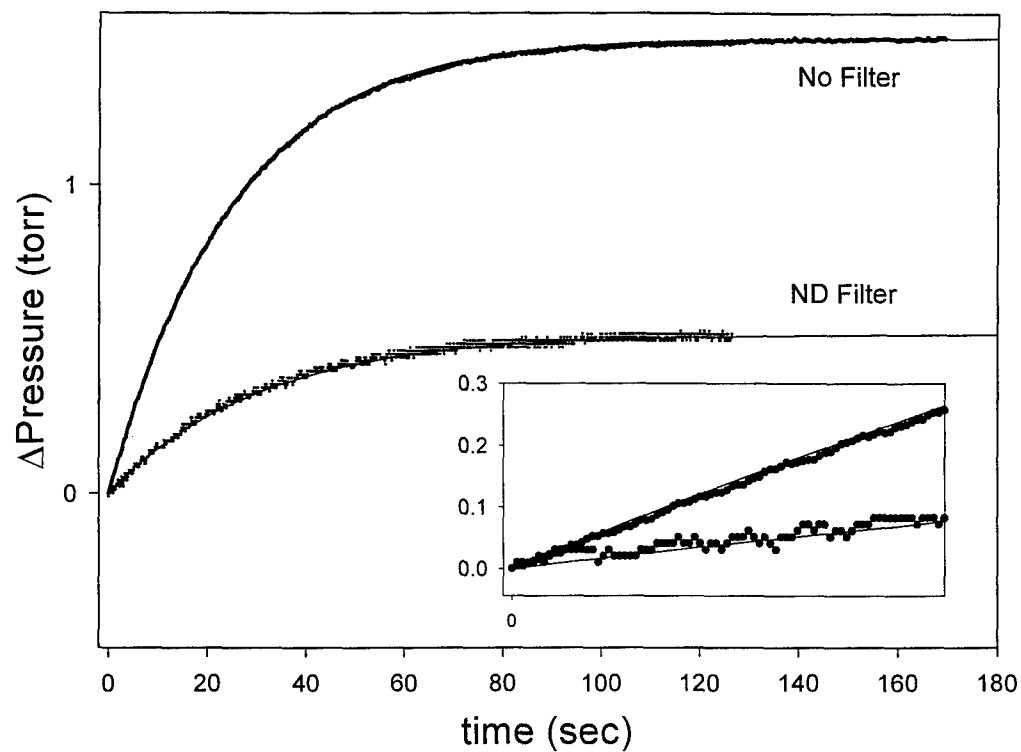


Figure 2.58 Comparison of pressure rise calculated from the light intensity, with and without a neutral density filter in place, to that predicted by the model;  $P_{eq}(\text{Br}_2) = .84$  torr,  $P_{eq}(\text{NO}) = 41.5$  torr,  $P_{eq}(\text{BrNO}) = 20.26$  torr.



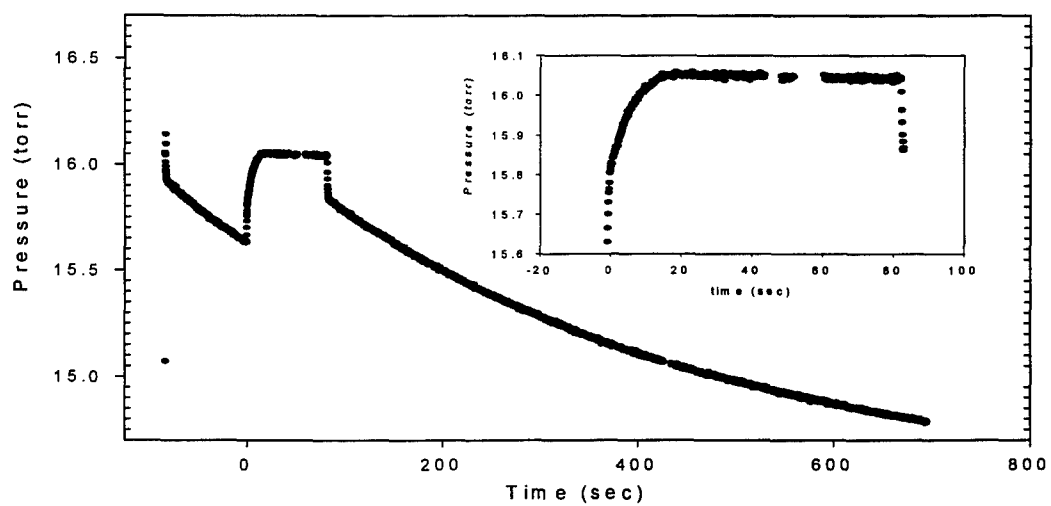


Figure 2.59 Pressure change after 4.0 torr of NO is added to 11.9 torr of Br<sub>2</sub> and shutter is opened. The mixture had not reached equilibrium when the shutter opened.

### *III. Spectroscopy*

Section 3.1 presents an overview of the history of spectroscopy. In Section 3.2 the quantum mechanical description of molecular rotation is discussed, the energies of a rigid rotor are found and the effects of non-rigidity determined. In the succeeding subsections the vibrational energy levels are described, the selection rules for the observed transitions are derived and the coupling of vibration and rotation discussed. Some useful approximations and relations are then presented. The most important result presented in this section is a Hamiltonian function (Equation 3.16, page 3-12) that gives the energy levels of a rotating non-rigid asymmetric molecule and is used to fit the experimental observations.

In Section 3.3 the theory and practice of Fourier transform spectroscopy are addressed. Section 3.4 reviews previous efforts along these lines and Section 3.5 describes the specific experimental and analytical techniques used in this experiment. The spectra are shown and their analysis discussed in Section 3.6. The chapter ends with a summary of this experiment and suggestions for future work.

#### *3.1 Overview of the Development of Spectroscopy*

Spectroscopy got its start in 1672 when Newton described his studies on the spectral dispersion of light rays by prisms but the field lay fallow until a burst of discoveries in the nineteenth century made it a useful analytical technique. In 1802 Wollaston observed a candle flame through a prism and noted the discontinuous nature of the spectrum. Using an improved prism, he distinguished dark absorption lines in the solar spectrum but ended this line of research after concluding that the lines were the boundaries between various colors of the spectrum. After constructing an exceptional prism for use in his efforts to perfect the achromatic lens, Fraunhofer rediscovered numerous dark lines in solar spectrum in 1814 and later measured the positions of over five hundred. He discovered that the reflected light from the moon,

Venus and Mars contains the same lines as those in the solar spectrum, while light from other stars contains different lines. In 1859 Kirchhoff realized that each chemical element, when heated to incandescence, produces its own characteristic pattern of colored lines and also realized (as did others at about the same time) that elements absorb at the same wavelengths as they emit when heated. Kirchhoff reasoned that the dark Fraunhofer lines are due to absorption of radiation by gases in the outer solar atmosphere. Bunsen and Kirchhoff made spectroscopy a sensitive tool for chemical analysis when they allowed light to pass through a slit before reaching their prism. The duo compared the solar spectrum with laboratory spectra of individual elements and established that hydrogen, nickel, iron, sodium, calcium, magnesium, barium, chromium, copper and zinc are present in the sun. They almost immediately discovered two new elements, cesium and rubidium, and named them for the color of the most prominent lines in their spectra, (sky-blue and red).

Infrared spectroscopy developed more slowly than visible spectroscopy. Herschel discovered infrared radiation in 1800 when he found an unexpected heating effect beyond the red end of the solar spectrum but it was almost a hundred years before Coblentz determined in 1892 that different atomic groupings absorb characteristic and specific wavelengths in the infrared. The detectors available to Coblentz, however, were too crude to convert his discovery into a useful analysis technique and infrared spectroscopy languished until the development of cooled detectors during WWII. Once sensitive detectors were available, IR spectroscopy rapidly matured into a useful tool.

### *3.2 Theory*

Absorption spectra result when a molecule shifts from a lower energy level to a higher one by absorbing a photon. The wavelength of the absorbed photon

corresponds to the energy difference between the two levels:

$$\Delta E = h\nu = \frac{hc}{\lambda} = hc\bar{\nu} \quad (3.1)$$

The allowed energy levels of a molecule are the eigenvalues of the time-independent Hamiltonian operator acting on the molecular wavefunction:

$$H \psi(\vec{r}) = E \psi(\vec{r}) \quad (3.2)$$

One approach to understanding the spectrum of a molecule is therefore the development of a Hamiltonian operator that gives the allowed energy levels at least as accurately as the energy levels can be determined from the spectrum.

A molecule possesses translational, electronic, rotational and vibrational energy. Analytical expressions for the energy levels can be derived once some simplifying assumptions are made. The Born-Oppenheimer approximation is often used to separate the electronic and nuclear wavefunctions of polyatomic molecules (8). The total wavefunction can be separated into translational, electronic, rotational and vibrational components to give

$$\psi_{total} = \psi_{trans} \psi_{elec} \psi_{rot} \psi_{vib} \quad (3.3)$$

and the total energy of the molecule is

$$E_{total} = E_{trans} + E_{elec} + E_{rot} + E_{vib} \quad (3.4)$$

Free translation is not quantized and therefore gives rise to a continuum of spectral lines. The rotational and vibrational energies of a molecule are quantized, as is the electronic energy of a molecule unless the molecule is in a dissociative state. Since this experiment investigated only infrared spectra, which involve transitions

between the rotational and vibrational levels of a single electronic state, electronic energy levels need not be discussed.

Another simplification assumes that the molecule is rigid—the relative positions of the atoms that comprise the rotating molecule are fixed. The vibrational motion can be treated by supposing that the nuclei execute small oscillations about their equilibrium positions. These assumptions must ultimately be modified to make the quantum mechanics agree with observations but they provide a useful starting point for a discussion of the energy levels of a rotating and vibrating molecule.

*3.2.1 Classification of Rigid Rotors.* A rigid body spinning freely in space has rotational energy equal to  $\frac{1}{2} I \omega^2$  where  $\omega$  is the rotation rate of the body and  $I$  is the moment of inertia with respect to the axis of rotation. More generally, the energy is a function of the principal moments of inertia  $I_x$ ,  $I_y$ , and  $I_z$ , which are the eigenvalues of the moment of inertia tensor and lie in the directions of the three body-fixed principal axes of the molecule. An axis of symmetry must be a principal axis and there will be a principal axis perpendicular to any plane of symmetry. The quantized energy levels of a molecule may be expressed in terms of the molecule's principal moments of inertia or in terms of the rotational constants, defined as

$$B_{\alpha} = \frac{h}{8\pi^2 c I_{\alpha}} \quad ; \alpha = x, y, z \quad (3.5)$$

with units of wavenumbers ( $\text{cm}^{-1}$ ) or, after multiplying by  $c$ , Hz. These rotational constants are usually written as  $A$ ,  $B$  and  $C$  with  $A \geq B \geq C$ . Since the allowed energy levels depend on the rotational constants, it is useful to use these constants or the corresponding moments of inertia to classify molecules (Table 3.1). Asymmetric rotors may be further classified using a unitless asymmetry parameter  $\kappa$  defined as

$$\kappa = \frac{2B - A - C}{A - C} \quad (3.6)$$

where  $\kappa$  varies between 1 (oblate symmetric top) and -1 (prolate symmetric top).

Table 3.1 Classification of molecules based on moments of inertia or rotational constants.

Spherical tops	$I_a = I_b = I_c$	$A = B = C$
Linear molecules	$I_a = 0, I_b = I_c$	$A = \infty, B = C$
Prolate symmetric tops	$I_a < I_b = I_c$	$A > B = C$
Oblate symmetric tops	$I_a = I_b < I_c$	$A = B > C$
Asymmetric rotors	$I_a < I_b < I_c$	$A > B > C$

Since the largest principal moment of inertia of a plane figure is the sum of the two smaller moments, a rigid plane molecule cannot be a spherical top or a prolate symmetric top. However, if  $I_a$  is small compared to  $I_b$  and  $I_c$  then  $I_c = (I_a + I_b) \approx I_b$  and the molecule is almost prolate. This is the case for nitrosyl bromide (Figure 3.1), a nonlinear molecule composed of an oxygen and a nitrogen atom and a much heavier bromine atom. The ground state asymmetry parameter is approximately -0.996 (Table 3.10) but varies depending on which isotopes of oxygen, nitrogen and bromine are incorporated into the molecule. (Naturally-occurring oxygen and nitrogen are composed almost entirely of  $^{16}\text{O}$  and  $^{14}\text{N}$ . The  $^{81}\text{Br}$  and  $^{79}\text{Br}$  isotopes each represent about half of the naturally-occurring bromine. Other, man-made isotopes of bromine are radioactive with halfives ranging from 1.6 seconds to 57 hours.) The  $c$  principal axis (corresponding to the largest moment of inertia) is perpendicular to the  $a$  (smallest moment) and  $b$  (intermediate moment) principal axes which lie in the plane of the molecule. From electron diffraction studies, the N-O bond length is 1.15 Å, the Br-N bond length is 2.14 Å, and the angle between the N-O and N-Br bonds is 117° (41).

**3.2.2 Rigid Rotor Energy Levels.** The total angular momentum  $\vec{J}$  of a freely rotating molecule is constant in direction and magnitude. In wavenumber

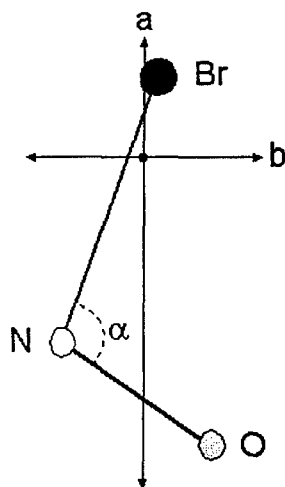


Figure 3.1 Schematic of BrNO structure.

units, the Hamiltonian of a rigid rotating molecule is

$$\hat{H}_{\text{rigid}} = B_x \hat{J}_x^2 + B_y \hat{J}_y^2 + B_z \hat{J}_z^2 \quad (3.7)$$

where  $\hat{J}_x$ ,  $\hat{J}_y$  and  $\hat{J}_z$  are the angular momentum operators in the molecule-fixed frame and  $\hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 = \hat{J}^2$ . The Hamiltonian may be reformulated to take advantage of any near symmetric top character present (40). The reformulated Hamiltonian is written as

$$\begin{aligned} \hat{H}_{\text{rigid}} = & \frac{1}{2}(B_x + B_y)\hat{J}^2 + [B_z - \frac{1}{2}(B_x + B_y)]\hat{J}_z^2 \\ & + \frac{1}{4}(B_x - B_y)[(\hat{J}_x + i\hat{J}_y)^2 + (\hat{J}_x - i\hat{J}_y)^2]. \end{aligned} \quad (3.8)$$

The quantum mechanical treatment of angular momentum shows that the rotational wavefunction of a molecule may be expanded using a set of basis vectors  $|j, k\rangle$  for which

$$J^2|j, k\rangle = \hbar^2 j(j+1)|j, k\rangle \quad (3.9)$$

$$J_z|j, k\rangle = \hbar k|j, k\rangle \quad (3.10)$$

The angular momentum component operators are subject to the commutation rule

$$[\hat{J}_\alpha, \hat{J}_\beta] = -i \sum_\gamma e_{\alpha\beta\gamma} \hat{J}_\gamma \quad (3.11)$$

where the minus sign appears because the angular momenta are referenced to the molecular axes, not the space-fixed axes. The effect of  $(J_x \mp i J_y)$ , the raising and lowering operators, are determined using Equations 3.9, 3.10 and 3.11 to be:

$$\begin{aligned} \langle J, k-1 | (\hat{J}_x + i\hat{J}_y) | J, k \rangle &= [J(J+1) - k(k+1)]^{1/2} \\ \langle J, k+1 | (\hat{J}_x - i\hat{J}_y) | J, k \rangle &= [J(J+1) - k(k-1)]^{1/2} \end{aligned}$$

The non-zero elements of the matrix derived using the reformulated Hamiltonian (Equation 3.9) are then

$$\begin{aligned} \langle J, k | \hat{H}_{\text{rigid}} | J, k \rangle &= \frac{1}{2}(B_x + B_y)J(J+1) + [B_z - \frac{1}{2}(B_x + B_y)]k^2 \quad (3.12) \\ \langle J, k \pm 2 | \hat{H}_{\text{rigid}} | J, k \rangle &= \frac{1}{4}(B_x - B_y)\{[J(J+1) - k(k \pm 1)] \\ &\quad \times [J(J+1) - (k \pm 1)(k \pm 2)]\}^{1/2} \quad (3.13) \end{aligned}$$

and diagonalizing this matrix gives the allowed rotational energy levels. The rotational constants  $B_x$ ,  $B_y$  and  $B_z$  can be matched to the A, B and C constants in six different ways (Table 3.2). The  $I^r$  orientation makes the off-diagonal terms in the Hamiltonian of a nearly prolate molecule as small as possible. The  $III^r$  orientation works best for nearly oblate tops while  $II^r$  minimizes the diagonal terms of the Hamiltonian of a highly asymmetric top. (The  $r$  and  $l$  versions of each orientation are the same except for the signs of the terms in the transformed Hamiltonian.) For a symmetric top with  $B_x = B_y$  the off-diagonal Hamiltonian matrix elements (Equation 3.13) are zero. Using the  $I^r$  orientation, the allowed energy levels of a prolate



Table 3.2 The six ways of identifying  $B_x$ ,  $B_y$ ,  $B_z$  with A, B, C.

	I <sup>r</sup>	II <sup>r</sup>	III <sup>r</sup>	I <sup>l</sup>	II <sup>l</sup>	III <sup>l</sup>
$B_x$	B	C	A	C	A	B
$B_y$	C	A	B	B	C	A
$B_z$	A	B	C	A	A	C

symmetric top are:

$$E_{\text{prolate}}(J, K) = BJ(J + 1) + (A - B)K^2 \quad (3.14)$$

Since nitrosyl bromide is almost prolate, its energy levels may reasonably be expected to be approximately those given by Equation 3.14. This approximation, used in the following sections to determine the rotational level populations and other quantities, is discussed more fully in Section 3.2.7.

Observable transitions involve rotational levels with  $J = 70$  and higher, making the matrix that must be diagonalized to find the energies of a rigid asymmetric rotor quite large. The task is made easier by reducing the matrix to a tridiagonal form using the Wang transformation, which takes advantage of the fact that the Hamiltonian matrix can be divided into submatrices that are symmetric about both diagonals and whose only nonzero elements are those for which  $k$  differs by 0 or  $\pm 2$ . There is a submatrix for each value of  $J$ , of dimension  $(2J + 1) \times (2J + 1)$ . The submatrices for  $J = 0, 1$  and  $2$  are illustrated in Figure 3.2. The tridiagonal matrix produced by the Wang transformation consists of interleaved odd and even  $K$  elements that may be further separated into four sub-blocks distinguished by the symmetry of the rotational levels whose energies are given by diagonalizing the sub-blocks (40). Diagonalization of the matrices gives  $2J + 1$  different energy levels for each value of  $J$ . Since there is in general no axis fixed to the molecule that carries out a simple rotation about  $\vec{J}$  there is no good quantum number having a definite physical meaning that distinguishes the different levels. In the symmetric rotor representation

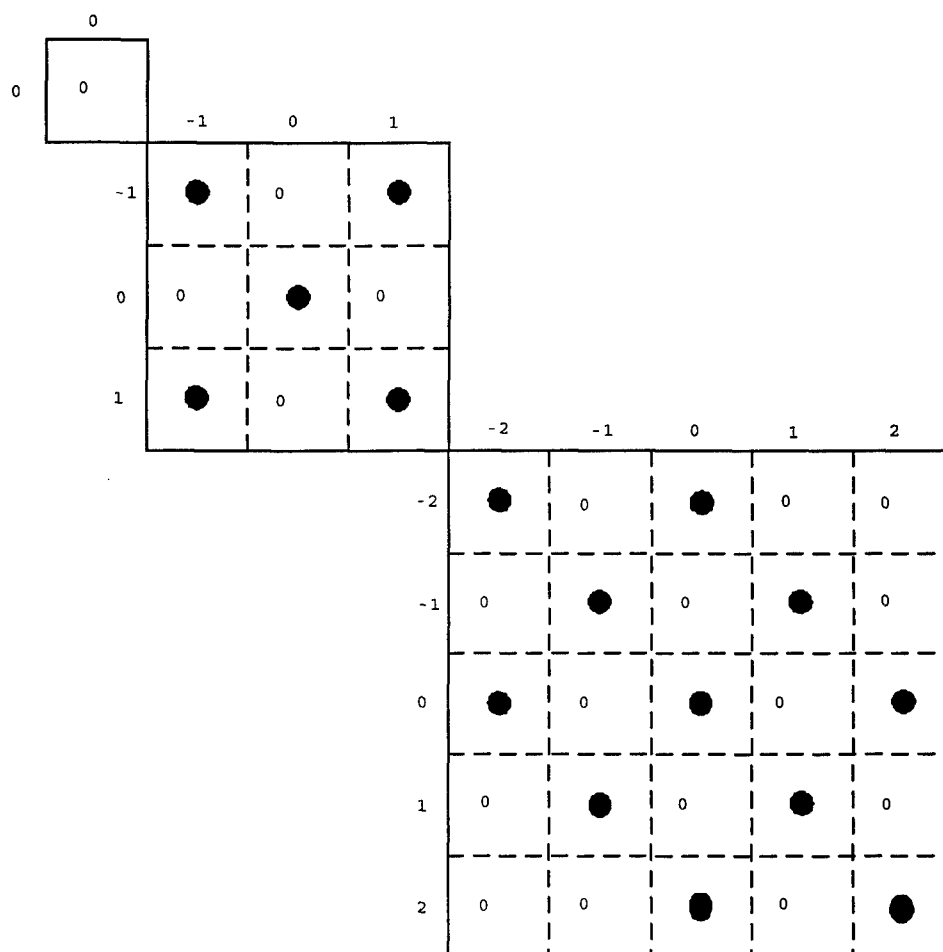


Figure 3.2 Rigid asymmetric top Hamiltonian matrix for  $J = 0, 1, 2$ . Elements labeled by  $k$ . Nonzero matrix elements shown by •.

the levels are designated by  $J_{K_a, K_c}$  where  $K_a$  is the value of  $K$  for the limiting prolate symmetric rotor ( $B = C$ ) with which the level correlates and  $K_c$  is the value of  $K$  in the oblate rotor limit ( $B = A$ ). This labeling scheme is illustrated in Figure 3.3. (Some authors use  $K_{-1}$  and  $K_{+1}$  instead of  $K_a$  and  $K_c$ . An older notation now rarely used labels the levels using  $\tau = K_a - K_c$ .) Since the energy increases with increasing  $K_a$  but decreases with increasing  $K_c$ , the energy levels for a given  $J$  in order of increasing energy are  $J_{0,J}, J_{1,J}, J_{1,J-1}, J_{2,J-1}, J_{2,J-2}, \dots, J_{J-1,2}, J_{J-1,1}, J_{J,1}, J_{J,0}$ .

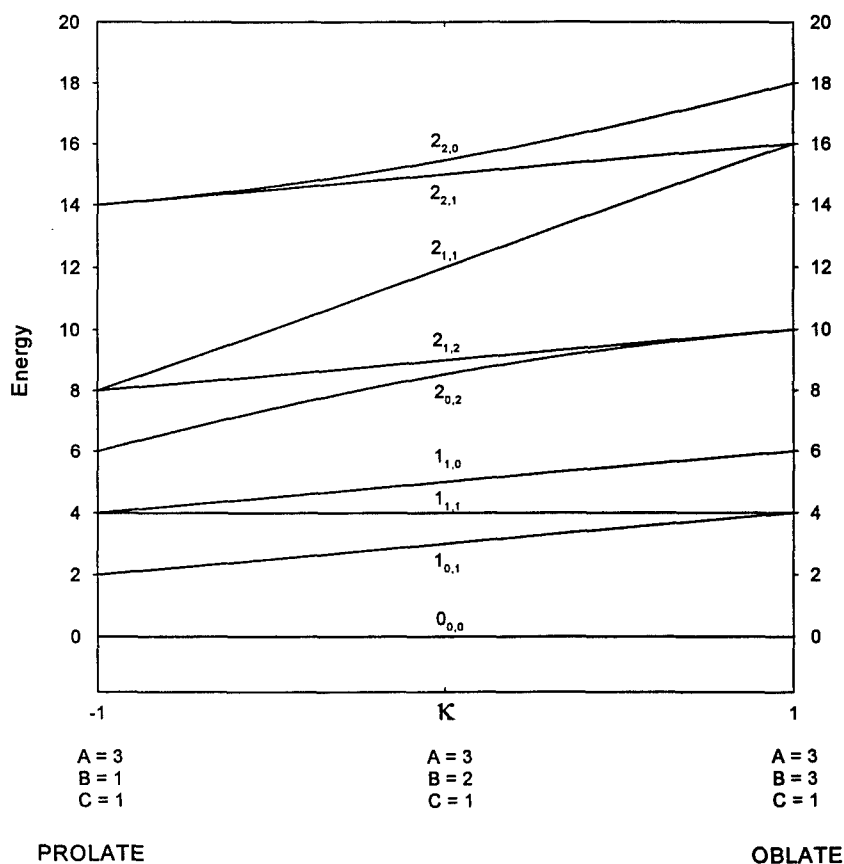


Figure 3.3 Rotational energy levels of asymmetric top molecules for  $J = 0, 1$  and  $2$  as a function of  $\kappa$ . The levels are labeled by  $J_{K_a, K_c}$ .

Explicit expressions for the rotational energy levels of rigid asymmetric top molecules have been tabulated. The energy of the  $3_{0,3}$  level, for instance, is given by

$$E(3_{0,3}) = 2A + 5B + 5C - 2\sqrt{4(B - C)^2 + (A - B)(A - C)} \quad (3.15)$$

Instead of looking up the tabulated energies, however, it is easier to determine the energy levels by numerically diagonalizing the Hamiltonian matrix for specific values of the rotational constants.

*3.2.3 Centrifugal Effects.* Since the bonds between real atoms are not rigid the centrifugal forces acting on the nuclei distort a rotating molecule. The moments of inertia vary for different rotational states and the energies of the states are not given by the rigid-rotor Hamiltonian. The analysis of high-resolution spectra therefore requires the development of a Hamiltonian that incorporates the distortion effects. The centrifugal distortion typically leads to small changes in the rotational energy levels and the first attempts at a quantum mechanical solution used perturbation methods. However, the resulting expressions were valid for only restricted ranges of  $J$  and did not adequately reproduce observed spectra.

The direct diagonalization of a rotational Hamiltonian that includes distortion effects requires fairly elaborate calculations and will only be outlined here. An article by Watson (67) and a book by Kroto (40) are excellent overviews and the sources for much of the following discussion.

The first step is to write the rotational Hamiltonian in a general form valid for all molecules with orthorhombic symmetry,

$$H_{rot} = \sum_{pqr} h_{pqr} (J_x^p J_y^q J_z^r + J_z^r J_y^q J_x^p)$$

The invariance of the Hamiltonian to Hermitian conjugation and time reversal forces the  $h$ 's to be real and to vanish if  $n = p + q + r$  is odd. The sum converges rapidly

because the terms with  $n = 2$  are typically much larger than the  $n = 4$  terms which in turn are much larger than the  $n = 6$  terms. The terms with  $n > 2$  are the centrifugal distortion constants.

If the Hamiltonian is truncated at sixth order in  $J$  the resulting equation contains nineteen constants but not all of these are independent. It may be transformed using Watson's "A" reduction to a form involving fifteen independent terms that can be determined from spectroscopic data:

$$\begin{aligned}
 H_{rot}^{(A)} = & B_x^{(A)} J_x^2 + B_y^{(A)} J_y^2 + B_z^{(A)} J_z^2 \\
 & - \Delta_J J^4 - \Delta_{JK} J^2 J_z^2 - \Delta_K J_z^4 \\
 & + \Phi_J J^6 + \Phi_{JK} J^4 J_z^2 + \Phi_K J_z^6 + \Phi_{KJ} J^2 J_z^4 \\
 & - \frac{1}{2} [(\delta_J J^2 + \delta_K J_z^2 - \phi_J J^4 - \phi_{JK} J^2 J_z^2 - \phi_K J_z^4), (J^+)^2 + (J^-)^2]_+
 \end{aligned} \tag{3.16}$$

where  $J^\pm = J_x \pm iJ_y$  and  $[X, Y]_+$  is the anticommutator  $XY + YX$ . The resulting Hamiltonian matrix elements (compare Equations 3.12 and 3.13) are

$$\begin{aligned}
 E_{k,k} = \langle J, k | \hat{H}_{rot}^{(A)} | J, k \rangle = & \frac{1}{2} [B_x^{(A)} + B_y^{(A)}] J(J+1) + \{B_z^{(A)} - \frac{1}{2} [B_x^{(A)} + B_y^{(A)}]\} k^2 \\
 & - \Delta_J J^2 (J+1)^2 - \Delta_{JK} J(J+1) k^2 - \Delta_K k^4 + \Phi_J J^3 (J+1)^3 \\
 & + \Phi_{JK} J^2 (J+1)^2 k^2 + \Phi_{KJ} J(J+1) k^4 + \Phi_K k^6
 \end{aligned} \tag{3.17}$$

$$\begin{aligned}
 E_{k\pm 2, k} = \langle J, k \pm 2 | \hat{H}_{rot}^{(A)} | J, k \rangle = & \left\{ \frac{1}{4} [B_x^{(A)} - B_y^{(A)}] - \delta_J J(J+1) \right. \\
 & - \frac{1}{2} \delta_K [(k \pm 2)^2 + k^2] + \phi_J J^2 (J+1)^2 \\
 & + \frac{1}{2} \phi_{JK} J(J+1) [(k \pm 2)^2 + k^2] + \frac{1}{2} \phi_K [(k \pm 2)^4 + k^4] \Big\} \\
 & \times \{ [J(J+1) - k(k \pm 1)] [J(J+1) - (k \pm 1)(k \pm 2)] \}^{\frac{1}{2}}
 \end{aligned} \tag{3.18}$$

The eigenvalues obtained by diagonalizing the resulting Hamiltonian matrix are the allowed rotational energies. The five  $\Delta_i$  and  $\delta_i$  coefficients represent the quartic effects of the centrifugal distortion while the seven  $\Phi_i$  and  $\phi_i$  terms quantify the

sextic effects. Since it is not practical to tabulate solutions, the energy levels must be found numerically. If the centrifugal distortion is large enough the  $J_{K_a, K_c}$  labeling scheme discussed in Section 3.2.2 may not order the energy levels correctly.

**3.2.4 Vibrational Energy Levels.** The bonds between atoms that allow rotating molecules to distort also permit the molecules to vibrate. The vibrational energy of a molecule is quantized and transitions may occur between rotational levels in two different vibrational levels. The resulting ro-vibrational spectra are observed in the infrared.

The vibrational motion of a molecule composed of  $n$  atoms can be described by the superposition of  $(3n - 6)$  fundamental vibrational modes if the molecule is nonlinear and  $(3n - 5)$  modes if it is linear. This partition of the vibration of a molecule into *normal modes* is an approximation that is strictly valid only if the vibrations are harmonic. Since BrNO is nonlinear it has three normal modes with frequencies (in  $\text{cm}^{-1}$ )  $\bar{\omega}_1$ ,  $\bar{\omega}_2$  and  $\bar{\omega}_3$ . The vibrational energy levels are labeled  $(v_1, v_2, v_3)$  according to the number of quanta in each mode. In an asymmetric rotor in general, there are no degenerate vibrational modes.

Just as the frequency of the simple harmonic motion of an object suspended by a spring depends on the spring constant and the mass of the object, the frequencies of the normal modes of a molecule are determined by the bonds between its atoms and by the masses of the atoms. The potential energy of a molecule can be expanded in a power series with respect to a complete and nonredundant set of internal displacement coordinates  $\{q_i\}$ :

$$V = \frac{1}{2} \sum_{i,j} F_{ij} q_i q_j + \frac{1}{6} \sum_{i,j,k} F_{ijk} q_i q_j q_k + \dots \quad (3.19)$$

where the internal coordinates are usually bond lengths and angles and the sums are taken over  $i, j = 1, 2, \dots, 3n - 6$  for nonlinear molecules. The completeness and nonredundance of the coordinates ensures that the expansion is unique (6). If

only the quadratic terms are considered, the sum gives a square matrix of  $F_{ij}$  values consisting of force constants on the diagonal plus symmetric off-diagonal interaction terms that may be negative and are often small. For BrNO, the resulting harmonic potential energy function is

$$V = \frac{1}{2} F_{NO}(q_{NO})^2 + \frac{1}{2} F_{NBr}(q_{NBr})^2 + \frac{1}{2} F_{\alpha}(q_{\alpha})^2 + F_{NO,NBr}(q_{NO})(q_{NBr}) + F_{NO,\alpha}(q_{NO})(q_{\alpha}) + F_{NBr,\alpha}(q_{NBr})(q_{\alpha}) \quad (3.20)$$

So that all the force constants have the same units, the angle bending coordinate  $q_{\alpha}$  frequently incorporates a fixed length  $R_0$ . To understand the significance of the interaction terms, consider the force acting to restore the angle between the N-O and N-Br bonds to its equilibrium value:

$$\text{Restoring force on } q_{\alpha} = -\frac{\partial V}{\partial q_{\alpha}} = F_{\alpha}q_{\alpha} + F_{NO,\alpha}q_{NO} + F_{NBr,\alpha}q_{NBr} \quad (3.21)$$

Without the interaction terms, the restoring force on the angle bending displacement would depend on the angular displacement but not on any simultaneous changes in the bond lengths. Each of the normal modes of an asymmetric rotor is a mixture of bond stretching and angle bending.

With only the quadratic terms included in the potential energy the quantized vibrational energy levels of a molecule are given by

$$E(v_1, v_2, v_3) = \left(v_1 + \frac{1}{2}\right) \omega_1 + \left(v_2 + \frac{1}{2}\right) \omega_2 + \left(v_3 + \frac{1}{2}\right) \omega_3 \quad (3.22)$$

This equation predicts that the energy levels are separated by integral multiples of the fundamental frequencies but spectroscopic data show that the vibrational levels become more closely spaced as  $v$  increases.

3.2.5 *Allowed Transitions and Line Strengths.* The absorption spectra considered here are produced by the interaction between light and the permanent dipole moment  $\vec{\mu}$  of BrNO molecules. The intensity (energy per unit area per second) of light with frequency  $\nu$  after it passes through a length  $x$  of absorbing gas is given by the Beer-Lambert relation:

$$I(\nu) = I_0 e^{-\gamma(\nu) x} \quad (3.23)$$

When a molecule absorbs a photon it jumps from a level labeled by the aggregate quantum number  $m$  to a higher one labeled by  $n$ ; the molecule then spontaneously emits a photon and returns to the lower level. As long as the population of the upper state is smaller than that of the lower state the balance between these processes causes a net loss in intensity. The absorption coefficient is

$$\gamma(\omega) = \frac{8\pi^3 \nu}{3hc} \left( \frac{N_m}{g_m} \right) \left( 1 - e^{-\beta (E_n - E_m)} \right) | \langle n | \vec{\mu} | m \rangle |^2 S(\nu, \nu_0) \quad (3.24)$$

where  $N_m$  is the concentration of molecules in the lower state and  $g_m$  is the degeneracy of the lower state;  $S(\nu, \nu_0)$  is a line shape function describing the broadening of the absorption line (Section 3.3.5);  $\langle n | \vec{\mu} | m \rangle$  is the dipole matrix element connecting the two states, and  $\beta = 1/kT$ . (At 298K,  $\beta$  is approximately  $4.83 \times 10^{-3}$  if the energy is in  $\text{cm}^{-1}$  and  $1.61 \times 10^{-7}$  if MHz are used.) The Boltzman factor appears because the concentrations of the lower and upper states are taken to be their equilibrium values.

The two factors that largely determine the intensity and positions of absorption lines—the magnitude of dipole matrix element connecting the upper and lower states and the population of the absorbing state—will be considered next.

3.2.5.1 *Dipole Matrix Elements.* If the dipole matrix element connecting the two states is zero the transition is not allowed. In the Born-Oppenheimer



approximation the vibrational and rotational parts of this term may be considered separately. The purely vibrational part determines the intensity of a ro-vibrational band relative to other bands and the rotational part determines the relative intensities of the lines within a given band.

The vibrational part of the dipole matrix is difficult to calculate when anharmonic effects are included. In the harmonic oscillator approximation the only allowed transitions are those in which a single vibrational quantum number changes by  $\pm 1$  but anharmonic effects allow weaker transitions between levels separated by more than one vibrational quantum (1). Since the anharmonic vibrational energy levels are not evenly spaced, the overtone transitions ( $v_i = 0 \rightarrow v_i = 2, 3, \dots$ ) of the fundamentals ( $v_i = 0 \rightarrow v_i = 1$ ) do not occur at integer multiples of the fundamental vibrations. A single photon may also excite more than one vibrational mode and the anharmonic effects produce combination band frequencies that are not equal to sums of integer multiples of the fundamental frequencies. The vibronic spectra of BrNO may be identified as  $n_1\nu_1 \pm n_2\nu_2 \pm n_3\nu_3$  bands where  $n_\alpha$  is the number of quanta gained or lost by each normal mode of vibration. The first overtone of the  $\nu_1$  vibration is then called  $2\nu_1$  while the hot band resulting from the transition from (0,1,0) to (1,0,0) is  $\nu_1 - \nu_2$ .

For asymmetric rotors the rotational part of the dipole matrix element is also quite difficult to calculate. Computer programs that perform this calculation are available (57) but the results cannot be summarized simply. However, by analyzing the symmetry of the rotational energy levels it is possible to specify when this term is nonzero and thereby determine which transitions are allowed.

Electric-dipole transitions between the rotational levels of all rotating quantum mechanical systems obey the rule

$$\Delta J = 0, \pm 1$$

with the restriction that transitions between two states with  $J = 0$  are forbidden. The three values of  $\Delta J$  produce spectra with a central Q branch ( $\Delta J = 0$ ) between an R branch ( $\Delta J = +1$ ) at lower wavelengths and a P branch ( $\Delta J = -1$ ) at larger wavelengths.

The rotational transitions of asymmetric top molecules are also restricted by selection rules for the  $K_a$  and  $K_c$  values. These rules depend on the orientation of the permanent dipole moment  $\mu$  relative to the principal axes of the molecule and the symmetries of the rotational levels, as shown in the following discussion.

The four submatrices produced by the Wang transformation (Section 3.2.2) are distinguished by the symmetry of the asymmetric rotor wave functions of the levels whose energies are given by diagonalizing the submatrices. Each submatrix, labeled  $E^\pm$  or  $O^\pm$ , has the symmetry  $\Gamma_{rot}$  of one of the irreducible representations A,  $B_a$ ,  $B_b$  and  $B_c$ . These representations reflect the result of the symmetry operation  $C_2^\alpha$ , a two-fold rotation about one of the principle axes of the molecule (Table 3.3).

Table 3.3 Character table for irreducible representations.

$\Gamma_{rot}$	I	$C_2^x$	$C_2^y$	$C_2^z$	Representation
ee	1	1	1	1	A
eo	1	1	-1	-1	$B_x$
oo	1	-1	1	-1	$B_y$
oe	1	-1	-1	1	$B_z$

The symmetry of the wavefunction associated with each rotational energy level and the submatrix the level belongs to may be determined by considering the parities of J,  $K_a$  and  $K_c$ , as shown in Table 3.4. The overall symmetry of the dipole term in Equation 3.24, given by the product of the symmetries of the initial and final states and the dipole component involved in the transition, must be A for an allowed transition. Since the a, b and c dipole moment components have symmetries  $B_a$ ,  $B_b$  and  $B_c$  respectively the allowed transitions occur between states of different symmetry and involve the components of the dipole moment shown in Table 3.5. Nitrosyl

Table 3.4 Symmetries of rotational energy levels in  $I^r$  representation. (e = even, o = odd)

J	$K_a$	$K_c$	submatrix	symmetry
e	e	e	$E^+$	A
e	e	o	$E^-$	$B_a$
e	o	e	$O^-$	$B_c$
e	o	o	$O^+$	$B_b$
o	e	e	$E^-$	A
o	e	o	$E^+$	$B_a$
o	o	e	$O^+$	$B_c$
o	o	o	$O^-$	$B_b$

Table 3.5 Component of dipole moment involved in transitions.

		final state			
		A	$B_a$	$B_b$	$B_c$
initial state	A	-	a	b	c
	$B_a$	a	-	c	b
	$B_b$	b	c	-	a
	$B_c$	c	b	a	-

bromide is a planar molecule and therefore cannot have a permanent dipole moment component along the  $c$  axis. Only transitions involving the  $a$  and  $b$  components are possible;  $a$ -type transitions involve  $ee \leftrightarrow eo$  or  $oe \leftrightarrow oo$  changes and obey the selection rule

$$\Delta K_a = 0, \pm 2, \dots \quad \Delta K_c = \pm 1, \pm 3, \dots$$

while  $b$ -type transitions are  $ee \leftrightarrow oo$  or  $oe \leftrightarrow eo$  and follow the selection rule

$$\Delta K_a = \pm 1, \pm 3, \dots \quad \Delta K_c = \pm 1, \pm 3, \dots$$

In the symmetric rotor representation the asymmetric wave functions are linear combinations of the symmetric wave functions. The wavefunctions of a slightly asym-

metric molecule are not mixed much and transitions in which  $K_a$  or  $K_c$  changes by more than  $\pm 1$  are very weak. The selection rules for strong transitions are then  $\Delta K_a = 0, \pm 1$  and  $\Delta K_c = \pm 1$  but the transitions are restricted further by the fact that the sum of  $K_a$  and  $K_c$  must be  $J$  or  $J + 1$  for both levels involved in the transition. The allowed transitions are listed in Table 3.6 along with additional restrictions specific to each transition. The last column of Table 3.6 lists a concise identification for each of the bands arising from the allowed transitions; the subscripts give  $\Delta K_a$  and  $\Delta K_c$  while the superscripts indicate the parity of the initial level and the type of transition. The sum  $J + K_a + K_c$  is even for a level with even parity and odd for an level with odd parity.

Table 3.6 Strong allowed transitions  $J_{K_a, K_c} \rightarrow J'_{K'_a, K'_c}$  for a nearly-prolate asymmetric top molecule.

$\Delta J$	$K_a + K_c$	$\Delta K_a$	$\Delta K_c$	Restrictions	Sub-branch
0	J	0	1	$K_a \neq 0$	$^{a,e}Q_{0,1}$
0	J	1	-1	$K_c \neq 0$	$^{b,e}Q_{1,\bar{1}}$
0	J	-1	1	$K_a \neq 0$	$^{b,e}Q_{\bar{1},1}$
0	J + 1	0	-1		$^{a,o}Q_{0,\bar{1}}$
0	J + 1	1	-1	$K_a \neq J$	$^{b,o}Q_{1,\bar{1}}$
0	J + 1	-1	1	$K_c \neq J$	$^{b,o}Q_{\bar{1},1}$
1	J	0	1		$^{a,e}R_{0,1}$
1	J	1	1		$^{b,e}R_{1,1}$
1	J + 1	0	1		$^{a,o}R_{0,1}$
1	J + 1	1	-1		$^{b,o}R_{1,\bar{1}}$
1	J + 1	-1	1		$^{b,o}R_{\bar{1},1}$
-1	J	0	-1	$K_c \neq 0$	$^{a,e}P_{0,\bar{1}}$
-1	J	1	-1	$K_c \neq 0, 1$	$^{b,e}P_{1,\bar{1}}$
-1	J	-1	1	$K_a \neq 0, 1$	$^{b,e}P_{\bar{1},1}$
-1	J + 1	0	-1	$K_a \neq J$	$^{a,o}P_{0,\bar{1}}$
-1	J + 1	-1	-1		$^{b,o}P_{\bar{1},\bar{1}}$

Since the dipole moment of BrNO is almost aligned along the  $a$  principal axis ( $\mu_a/\mu_b \approx 20$ )  $a$ -type ( $\Delta K_a = 0$ ) transitions dominate the absorption spectrum (12) but weaker  $b$ -type ( $\Delta K_a = \pm 1$ ) transitions have also been observed (13).

3.2.5.2 *Initial level populations.* The intensity of an absorption line also depends on the population of absorbing molecules. Under equilibrium conditions the Boltzman distribution gives for the fractional population of state m

$$\frac{N_m}{N} = \frac{g_m}{Q} \exp[-\beta E_m]$$

where Q is the partition function of the molecule and  $E_m$  is energy of state m above the ground state. If the rotational and vibrational energies are independent the total energy of a state is  $E_{vib} + E_{rot}$  and  $Q = Q_{vib} Q_{rot}$  so the fractional concentration is

$$\frac{N_m}{N} = \frac{g_m}{Q_{vib} Q_{rot}} \exp[-\beta E_m]_{rot} \exp[-\beta E_m]_{vib}$$

The normal modes of BrNO are not degenerate and the fractional concentration of BrNO molecules in state  $(v_1, v_2, v_3)$  is

$$\frac{N(v_1, v_2, v_3)}{N} = \frac{1}{Q_{vib}} \exp[-\beta hc(v_1 \nu_1 + v_2 \nu_2 + v_3 \nu_3)]$$

where the vibrational partition function is (40)

$$Q_{vib} = [(1 - e^{-\beta \nu_1})(1 - e^{-\beta \nu_2})(1 - e^{-\beta \nu_3})]^{-1}$$

The normal frequencies of  $^{16}\text{O}^{14}\text{N}^{79}\text{Br}$  (see Table 3.8) are about 1832, 548 and 270  $\text{cm}^{-1}$ . The vibrational partition function at 298 K and 1000K is

$$Q_{vib}(298K) = 1.49$$

$$Q_{vib}(1000K) = 6.27$$

The energies of the lower BrNO vibrational levels (41) are shown in Figure 3.4. The many near-degeneracies occur because  $\nu_2$  is approximately twice  $\nu_3$ . The fractional populations for these levels at 298K and 1000K are given in Table 3.7. Most of the

transitions observed in the room temperature infrared spectrum are due to transitions out of the highly populated ground state but weaker transitions out of the (0,1,0) and (0,0,1) levels are also seen. At higher temperatures the populations of the levels above the ground state increase and the spectra due to transitions out of those levels become more intense. Such spectra are, therefore, called *hot bands*.

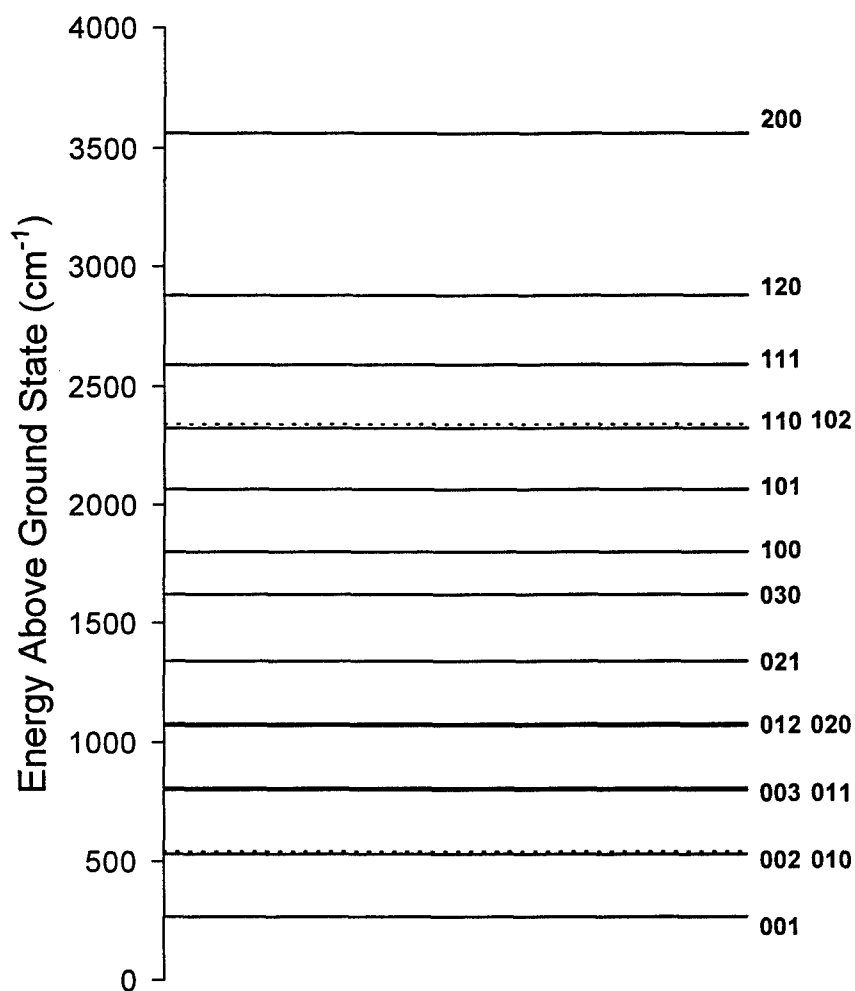


Figure 3.4 Lower vibrational levels of BrNO.

Table 3.7 Ratio of populations of lower BrNO vibrational levels to total number of molecules at 298K and 1000K.

Vibrational Level	298K	1000K
(0,0,0)	.6710	.159
(1,0,0)	.00011	.009
(0,1,0)	.049	.067
(0,0,1)	.186	.103
(0,0,2)	.051	.068
(0,2,0)	.0037	.028
(0,1,1)	.014	.043
(1,0,1)	.00003	.008
(1,1,0)	.000008	.006
(0,1,2)	.0037	.028
(1,2,0)	.0000006	.0016
(0,2,1)	.0010	.018
(0,0,3)	.014	.050
(0,3,0)	.00027	.012
$\Sigma$	.994	.601

The rotational contribution to the fractional concentration for the (J,K) level of a prolate symmetric top molecule is

$$\begin{aligned}
 \frac{N(J, K)}{N} &= \frac{g_I(K)}{Q_{rot}} (2J + 1) \exp \left\{ -\beta \left[ BJ(J + 1) + (A - B)K^2 \right] \right\} \\
 &= \frac{1}{Q_{rot}} \left\{ g_I(K) \exp \left[ -\beta (A - B)K^2 \right] \right\} \\
 &\quad \times \left\{ (2J + 1) \exp \left[ -\beta BJ(J + 1) \right] \right\} \quad (3.25)
 \end{aligned}$$

Where  $g_m = 2J + 1$  is the degeneracy of the ground state rotational levels arising from the quantization of  $J_z$  referenced to space-fixed axes. The nuclear spin degeneracy factor  $g_I(K)$  depends on the symmetry of the molecule and leads to a regular intensity variation in the ro-vibrational spectra. The rotational partition function of an asymmetric top molecule when  $E_{rot}$  is much less than  $kT$  is approximately (40)

$$Q_{rot} = \left[ \frac{\pi}{ABC\beta^3} \right]^{\frac{1}{2}} \quad (3.26)$$

The BrNO ground state rotational constants (13) are about 85500, 3730 and 3575 MHz and the rotational partition function at 298K is  $2.6 \times 10^4$ . The distribution of the populations of the rotational levels of  $^{79}\text{BrNO}$  at 298K, using the prolate symmetric top energy levels and ignoring the spin degeneracy, is shown in Figure 3.5. The maximum population occurs in about the  $J = 30$  level. The K-dependent part of Equation 3.25 scales the J-dependent part so the populations of levels with the same J decrease as K increases.

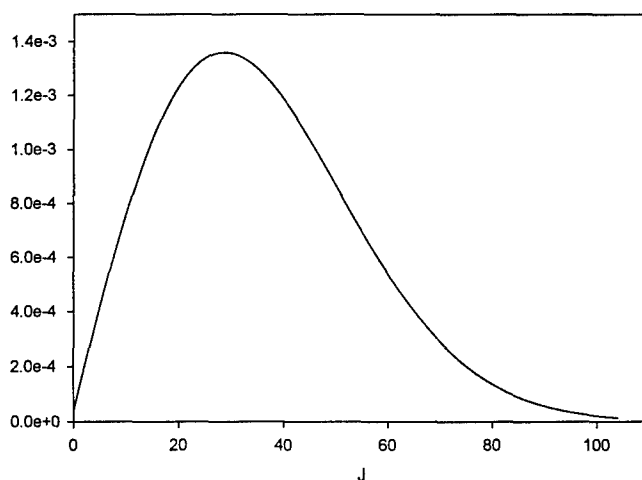


Figure 3.5 BrNO rotational line populations at 298K for  $K = 0$ .

**3.2.6 Coupling of Rotation and Vibration.** The vibration and rotation of the molecule are not truly independent. If a Morse potential is used to describe the vibrations of a rotating diatomic molecule, the molecular energy is

$$E(v, J) = \left(v + \frac{1}{2}\right) \bar{\omega} - \left(v + \frac{1}{2}\right)^2 \bar{\omega} x_e + \bar{B}_e J(J+1) - \bar{D} J^2 (J+1)^2 - \bar{\alpha}_e \left(v + \frac{1}{2}\right) J(J+1)$$

The  $\bar{\alpha}_e$  term represents the interaction of vibration and rotation. Since it has the same J dependence as the  $\bar{B}_e$  term the two can be combined into an effective rota-



tional constant that differs for each vibrational level. This procedure also works for polyatomic molecules and the rotation constants of a triatomic molecule to second order in  $v$  are written in the form (46)

$$B^v = B_e - \sum_i \alpha_i^B (v_i + \frac{1}{2}) + \sum_{i \geq j} \gamma_{ij}^B (v_i + \frac{1}{2})(v_j + \frac{1}{2}) + \dots \quad (3.27)$$

where the sums are taken over  $i = 1, 2, 3$ . The  $\alpha_i^B$  constants are generally about  $10^{-2}$  times the corresponding rotational constants while the  $\gamma_{ij}^B$  constants are another factor of 100 smaller and therefore usually ignored. Although the centrifugal distortion terms are also functions of the vibrational levels, the Hamiltonian for a non-rigid molecule (Equation 3.16) discussed in Section 3.2.3 remains valid.

The spectra due to transitions between the rotational levels of a molecule are found in the microwave or far-infrared, at frequencies of 50 to 200 GHz. The rotational constants for each level may be determined by analyzing these pure rotation spectra; however, the room-temperature populations (Section 3.2.4) of levels above the ground state are low and the rotational spectra of those levels are much weaker than the rotational spectrum of the ground state. The ro-vibrational transitions out of the highly-populated ground state are usually much stronger than the rotational spectra and their analysis provides an alternative method of determining the rotational constants of the higher states.

*3.2.7 Symmetric Top Approximations.* Since nitrosyl bromide is only slightly asymmetric its spectrum resembles that of a prolate symmetric top molecule. In this section several symmetric-top approximations are presented and the energy levels and spectra of prolate molecules are discussed.

In Section 3.2.2 the energy levels of a rigid prolate symmetric top were shown to be

$$E_{\text{prolate}}(J, K) = BJ(J+1) + (A-B)K^2 \quad (3.28)$$

The  $2J + 1$  different energy levels for each value of  $J$  for an asymmetric molecule are reduced to  $J$  two-fold degenerate levels and a single nondegenerate level for  $K = 0$ . The first effect of slight asymmetry is to split the degenerate levels. The trend shown in Figure 3.3 (Page 3-10), that the resulting  $K$ -type doubling increases with increasing  $J$  but decreases with increasing  $K$ , holds for higher  $J$  values. The splitting of the  $K \neq 1$  levels involves second or higher order terms only and is much smaller than the  $K = 1$  splitting (40). The energy levels of the split  $K = 1$  lines are approximately

$$E'(J, 1) = E(J, 1) \pm \frac{1}{4}(B - C)J(J + 1) \quad (3.29)$$

At low  $J$  values, these approximations are quite accurate for BrNO, which is very nearly prolate. With  $A = 85500$  MHz,  $B = 3747$  MHz and  $C = 3586$  Mhz (values close to those for the ground state of BrNO), the exact solution gives  $E(4_{1,3}) = 5.198929 \text{ cm}^{-1}$  and  $E(4_{1,4}) = 5.145263 \text{ cm}^{-1}$ . The approximate energies of these levels are  $5.1989505 \text{ cm}^{-1}$  and  $5.1452835 \text{ cm}^{-1}$ . Higher order corrective terms have been tabulated and may be added to maintain the accuracy of the approximations at higher  $J$  values.

The approximations for the energy levels of a nearly-prolate molecule are useful aids in the assignment of the ro-vibrational spectra of BrNO and may be used to check the output of the fitting program (Section 3.6.2). For BrNO the sum of the vibrational and rotational energies (without the  $K$ -splitting for the  $K_a = 1$  levels or the distortion terms) is

$$\begin{aligned} E(J, K_a, v_1, v_2, v_3) = & B_{avg}J(J + 1) + (A - B_{avg})K_a^2 \\ & + (v_1 + \frac{1}{2})\nu_1 + (v_2 + \frac{1}{2})\nu_2 + (v_3 + \frac{1}{2})\nu_3 \end{aligned} \quad (3.30)$$

For transitions from the  $(v_1, v_2, v_3)$  vibrational level to the  $(v'_1, v'_2, v'_3)$  level with  $\Delta J = 1$  and  $\Delta K_a = 0$  the positions of the spectral lines are

$$\begin{aligned}\Delta E(J, K_a, \nu_0) = & (B_{avg}^1 - B_{avg}^0)J^2 + (3B_{avg}^1 - B_{avg}^0)J + 2B_{avg}^1 \\ & + [(A^1 - A^0) - (B_{avg}^1 - B_{avg}^0)]K_a^2 \\ & + (v'_1 - v_1)\nu_1 + (v'_2 - v_2)\nu_2 + (v'_3 - v_3)\nu_3\end{aligned}\quad (3.31)$$

The sum  $(v'_1 - v_1)\nu_1 + (v'_2 - v_2)\nu_2 + (v'_3 - v_3)\nu_3 = \nu_0$  is called the band origin and is the same for all three branches of a given ro-vibrational band spectrum. It varies for isotopomers because different masses change the normal mode frequencies.

For Q branch transitions with  $\Delta J = 0$ ,  $\Delta K_a = 0$ , the positions of the lines are given by

$$\Delta E(J, K_a, \nu_0) = \nu_0 + (B_{avg}^1 - B_{avg}^0)J(J+1) + [(A^1 - A^0) - (B_{avg}^1 - B_{avg}^0)]K_a^2 \quad (3.32)$$

and for P branch transitions with  $\Delta J = -1$ ,  $\Delta K = 0$ ,

$$\Delta E(J, K_a, \nu_0) = \nu_0 + (B_{avg}^1 - B_{avg}^0)J^2 - (B_{avg}^1 + B_{avg}^0)J + [(A^1 - A^0) - (B_{avg}^1 - B_{avg}^0)]K_a^2 \quad (3.33)$$

The lines may be grouped into sub-bands or K-blocks consisting of transitions with the same  $K = K_a$  value and  $J = K, K + 1, \dots$ . Since the J-dependent part of the approximate transition frequency is independent of the K-dependent part, the patterns of the lines in each K-block are the same with the spacing between sub-bands determined by the K-dependent part. (These patterns are disrupted by distortion effects.) The distances separating successive transitions within each sub-band, called the second differences, are useful guides when assigning transitions. For R branch transitions

$$\Delta_J = \Delta E(J+1, K_a) - \Delta E(J, K_a)$$

$$= (B_{avg}^1 - B_{avg}^0)(2J + 1) + 3B_{avg}^1 - B_{avg}^0 \quad (3.34)$$

For the Q branch

$$\Delta_J = 2(B_{avg}^1 - B_{avg}^0)(J + 1) \quad (3.35)$$

and for the P branch

$$\Delta_J = 2J(B_{avg}^1 - B_{avg}^0) - 2B_{avg}^0 \quad (3.36)$$

The separation between the sub-bands for  $K_a$  and  $K_a + 1$  is

$$\Delta_K = [(A^1 - A^0) - (B_{avg}^1 - B_{avg}^0)](2K_a + 1). \quad (3.37)$$

The dipole term for a symmetric top is proportional to M, given by (1)

$$\begin{aligned} \frac{(2 - \delta_{K,0})(J + K + 1)(J - K + 1)}{J + 1} & ; \quad \Delta J = 1 \\ \frac{(2 - \delta_{K,0})(2J + 1)K^2}{J(J + 1)} & ; \quad \Delta J = 0 \\ \frac{(2 - \delta_{K,0})(J^2 - K^2)}{J} & ; \quad \Delta J = -1 \end{aligned}$$

where the Kronecker delta accounts for the two-fold degeneracy of the  $K \neq 0$  levels.

The relative values of the absorption coefficient within a single ro-vibrational band are obtained by ignoring all of the constant terms in Equation 3.24. For a transition out of the (J,K) rotational level of the (i j k) vibrational state the absorption coefficient is

$$\begin{aligned} \gamma(\nu)^{rel} &= \nu \exp\{-\beta[B_{avg}^{ijk}J(J + 1) + (A^{ijk} - B_{avg}^{ijk})K^2]\} \\ &\times \{1 - \exp(-\beta\nu)\} M S(\nu, \nu_0) \end{aligned} \quad (3.38)$$

The  $[1 - \exp(-\beta\nu)]$  term is almost unity for ro-vibrational transitions and varies little over the width of a single band.

The line intensities are modified by the nuclear spin degeneracy factor. For symmetric top  $C_{3v}$  molecules with  $I = 3/2$  in a given R branch K block the lines for  $K = 3, 6, \dots$  are stronger than the others in the ratio 6:5 (40).

*3.2.8 Planarity Relations.* The largest principal moment of inertia of a rigid planar object is equal to the sum of the two smaller moments of inertia but this restriction does not hold exactly for vibrating planar molecules (40). The inertial defect, defined as

$$\Delta^v = I_c^v - I_b^v - I_a^v \quad (3.39)$$

is usually a strong function of the vibrational quantum number. For the ground vibrational state of 'well-behaved' planar molecules  $\Delta^0$  is usually a small positive number (0.05 - 0.5 amu  $\text{\AA}^2$ ). (If the rotational constant is in MHz, multiply its reciprocal by 505391.307 to get amu  $\text{\AA}^2$ .) A negative value indicates that the molecule undergoes significant non-planar motion. Since the inertia defect is usually small, the relationship between the moments of inertia for a rigid plane molecule may guide the selection of rotational constants when spectral lines are being fitted.

Similar planarity relations exist between the equilibrium values of the centrifugal constants. For the A reduction and  $I^r$  representation, the relations (68) for a rigid molecule are

$$4C\Delta_J - (B - C)\Delta_{JK} - 2(2A + B + C)\delta_J + 2(B - C)\delta_K = 0, \quad (3.40)$$

$$\begin{aligned} 6C\Phi_J - (B - C)\Phi_{JK} - 2(2A + B + 3C)\phi_J + 2(B - C)\phi_{JK} \\ + 4\Delta_J^2 - 4\delta_J(4\Delta_J + \Delta_{JK} - 2\delta_J - 2\delta_K) = 0 \end{aligned} \quad (3.41)$$

Like the relationship between the moments of inertia, these equations only hold approximately for non-rigid molecules. The defect in the quartic relation may be large but the defect in the sextic relationship is usually insignificant.

### 3.3 *Fourier Transform Infrared Spectroscopy*

This section presents an overview of the theory and operation of a Fourier transform infrared (FTIR) spectrometer. More extensive discussions along with rigorous derivations of the pertinent equations can be found in the references.

*3.3.1 Background.* Fourier transform spectrometers are based on interferometers fundamentally identical to those designed and built by Michelson as early as 1880. Although his research establishing the constancy of the speed of light is better known, Michelson also recognized that his interferometer could be used as a spectrometer. He could not, however, develop the field due to the lack of appropriate detectors and other prerequisite technology. The first true interferogram was not recorded until 1911 by Rubens and Wood.

During WWII sensitive (cryogenically-cooled) infrared detectors and infrared spectrophotometers using gratings and prisms were developed. Shortly after the war the theoretical advantages of FT spectroscopy relative to dispersive techniques (especially in the FIR region) were recognized by Jacquinot, Fellgett and others and in the early 1950's experimenters at Johns Hopkins University showed that the theoretical advantages of FT spectroscopy could be achieved in practice. Later work at the Air Force Cambridge Research Center refined and extended the techniques developed at Johns Hopkins.

The pace of FT spectrometer development accelerated in the 1960s and today FTIR spectrometers are used throughout industry and research. Affordable spectrometers using microcomputers have been developed by various companies and have largely supplanted grating spectrophotometers, particularly for IR applications.

FT spectrometers have been lofted by balloon and have been part of many space missions, including the Viking missions to Mars.

*3.3.2 Theory.* The heart of the FTIR spectrometer used in this experiment, and the basis for most of the interferometric spectrometers in use today, is a Michelson interferometer (Figure 3.6), which divides a collimated beam of radiation into two paths and then recombines the beams after a variable path difference has been introduced. The diameter and divergence of the initial beam is set by the entrance aperture and the collimation optics. A detector measures the intensity of the recombined beam after it passes through a sample chamber. (For some purposes, the sample chamber is placed in one arm of the interferometer instead of in the path of the recombined beams.) The two beams interfere when recombined. If

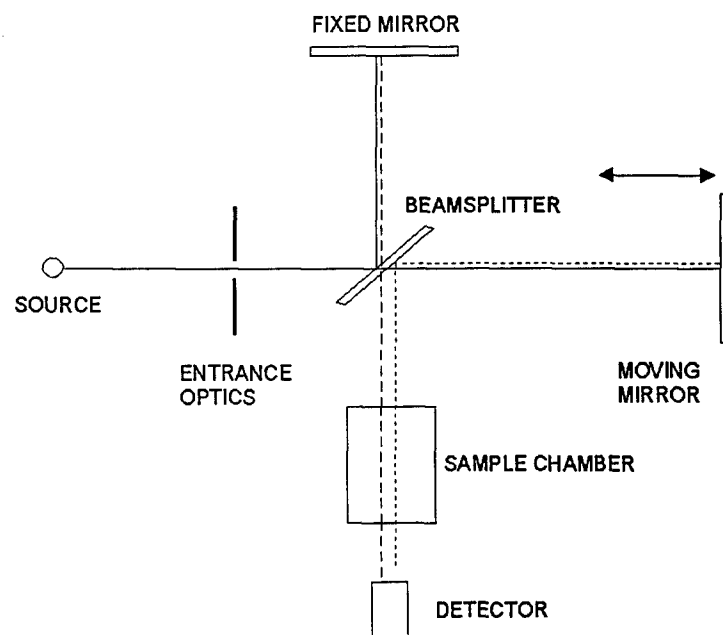


Figure 3.6 Schematic of Michelson Interferometer.

the source produced light with a single wavelength the output of the detector would vary sinusoidally with the change in path length. Maxima would occur when the

optical paths differed by integral multiples of the wavelength while minima would occur when the combining wavefronts were exactly out of phase.

In the general case, the source produces a continuous range of frequencies. The radiation entering the interferometer has intensity  $I_0$  described in terms of the electric field component of the radiation as:

$$I_0 = \langle \vec{E}(\vec{r}, t)^* \cdot \vec{E}(\vec{r}, t) \rangle \quad (3.42)$$

where  $\langle \rangle$  represents the time average  $\frac{1}{T} \int_0^T$  taken for  $T \rightarrow \infty$  and  $*$  is the complex conjugate. Assuming a planar wave, the electric field component wave may be expressed in terms of the frequencies present as:

$$\vec{E}(\vec{r}, t) = \int_{-\infty}^{+\infty} \sqrt{B(\nu)} e^{2\pi i(\nu t + \vec{r} \cdot \vec{\sigma})} d\nu \quad (3.43)$$

where  $\sqrt{B(\nu)}$  is the amplitude of the frequency component  $\nu$  and  $\sigma = \nu/c$  in the direction of propagation. Squaring the amplitudes of the frequency components gives the power spectral density  $B(\nu)$  which is the spectrum of the beam.

When the returned beams in the interferometer are superimposed at the beam-splitter, an output beam of radiation is produced consisting of the sum of the two electric field components. If the initial beam is split into two equal beams and the reflectances and transmissivities of the beamsplitter and mirrors are ignored, the sum is:

$$\vec{E}_{\text{out}}(\vec{r}, t) = \frac{\vec{E}(\vec{r}, t)}{2} + \frac{\vec{E}(\vec{r}, t + \tau)}{2} \quad (3.44)$$

where  $\tau$  is the difference in propagation time for the two separated beams. When the interferometer is accurately aligned, the superposition of the two returned beams is very precise and the electric fields of the two beams interact giving an output



intensity equal to:

$$I_{\text{out}} = \left\langle \left[ \frac{\vec{E}(\vec{r}, t)}{2} + \frac{\vec{E}(\vec{r}, t + \tau)}{2} \right]^* \cdot \left[ \frac{\vec{E}(\vec{r}, t)}{2} + \frac{\vec{E}(\vec{r}, t + \tau)}{2} \right] \right\rangle \quad (3.45)$$

Assuming that the time average is independent of the choice of the origin of time and that the vectorial nature of the optical fields can be ignored, Equation 3.45 gives:

$$I_{\text{out}} = \frac{1}{T} \int_0^T \left[ \frac{\vec{E}(\vec{r}, t)^*}{2} \cdot \frac{\vec{E}(\vec{r}, t)}{2} + \frac{\vec{E}(\vec{r}, t + \tau)^*}{2} \cdot \frac{\vec{E}(\vec{r}, t + \tau)}{2} + \frac{\vec{E}(\vec{r}, t)^*}{2} \cdot \frac{\vec{E}(\vec{r}, t + \tau)}{2} + \frac{\vec{E}(\vec{r}, t + \tau)^*}{2} \cdot \frac{\vec{E}(\vec{r}, t)}{2} \right] dt. \quad (3.46)$$

The first two terms in Equation 3.46 are the same as Equation 3.42 in the limit when  $T \gg \tau$ . Using Equation 3.43 to express  $\vec{E}(\vec{r}, t)$  in terms of  $B(\nu)$  gives:

$$\begin{aligned} I_{\text{out}} &= \frac{I_0}{4} + \frac{I_0}{4} + \frac{1}{T} \int_0^T \left[ \frac{\vec{E}(\vec{r}, t)^*}{2} \cdot \frac{\vec{E}(\vec{r}, t + \tau)}{2} + \frac{\vec{E}(\vec{r}, t + \tau)^*}{2} \cdot \frac{\vec{E}(\vec{r}, t)}{2} \right] dt \\ &= \frac{I_0}{2} + \frac{1}{T} \int_0^T \int_{-\infty}^{+\infty} \frac{B(\nu)}{4} [e^{-2\pi i(\nu t + \vec{r} \cdot \vec{\sigma})} \cdot e^{2\pi i(\nu(t + \tau) + \vec{r} \cdot \vec{\sigma})} + \\ &\quad e^{-2\pi i(\nu(t + \tau) + \vec{r} \cdot \vec{\sigma})} \cdot e^{2\pi i(\nu t + \vec{r} \cdot \vec{\sigma})}] d\nu dt \end{aligned} \quad (3.47)$$

and manipulating the exponential terms gives:

$$\begin{aligned} I_{\text{out}} &= \frac{I_0}{2} + \frac{1}{T} \int_0^T \int_{-\infty}^{+\infty} \frac{B(\nu)}{4} [e^{2\pi i\nu\tau} + e^{-2\pi i\nu\tau}] d\nu dt \\ &= \frac{I_0}{2} + \int_{-\infty}^{+\infty} \frac{B(\nu)}{2} \cos(2\pi\nu\tau) d\nu \end{aligned} \quad (3.48)$$

This can be written in terms of the optical path retardation,  $x$ , which corresponds to twice the displacement of the moving mirror. Since  $\bar{\nu} = \nu/c$  and  $x = c\tau$ ,

$$I_{\text{out}} - \frac{I_0}{2} = \int_0^{+\infty} B(\bar{\nu}) \cos(2\pi\bar{\nu}x) d\bar{\nu} \quad (3.49)$$

where the power spectral density is assumed to be an even function of  $\bar{\nu}$ . This, the fundamental equation of Fourier transform spectroscopy, shows that the output intensity minus half the input intensity is the Fourier cosine transform of the spectrum. Since the Fourier transform is invertible, the spectrum can be obtained by performing an inverse cosine Fourier transform on  $C(x) = I_{\text{out}} - I_0/2$ :

$$B(\bar{\nu}) = \int_0^{+\infty} C(x) \cos(2\pi\bar{\nu}x) \, dx. \quad (3.50)$$

Determining  $C(x)$ , the *interferogram*, at the output of the interferometer as a function of the path difference between the two arms of the interferometer, therefore, allows the determination of the intensity of the recombined beams as a function of wavenumber. Since this intensity is modified when the recombined beam passes through the sample, the spectrum of the sample may also be determined.

The above result assumes no phase difference between the recombining beams, but such error is always present because of misalignment of the interferometer, dispersion by the beamsplitter, and errors in data acquisition. This error manifests itself as asymmetry in the interferogram but may be corrected during processing using phase information obtained before the interferogram is captured (45).

The form of  $C(x)$  for various inputs can be determined using Equation 3.49 or by reference to a table of Fourier transform pairs, remembering that  $B(\bar{\nu})$  is real and even. When the input beam has only a single component at  $\bar{\nu}_0$  the interferogram is

$$C(x) = B(\bar{\nu}_0) \cos(2\pi\bar{\nu}_0x). \quad (3.51)$$

This corresponds to using a laser as the input and provides a way to monitor the movement of the mirror by counting zero crossings in the resulting interferogram. The interferogram of a quasi-monochromatic source is a cosine with gradually diminishing amplitude.

The Fourier transform is a linear function. Therefore, for an input composed of two equal single-frequency components at  $\bar{\nu}_1$  and  $\bar{\nu}_2$  the interferogram is the sum of two terms like Equation 3.51:

$$\begin{aligned} C(x) &= B(\bar{\nu}_{1,2})\{\cos(2\pi\bar{\nu}_1x) + \cos(2\pi\bar{\nu}_2x)\} \\ &= 2 B(\bar{\nu}_{1,2}) \cos[\pi(\bar{\nu}_1 + \bar{\nu}_2)x] \cos[\pi(\bar{\nu}_1 - \bar{\nu}_2)x]. \end{aligned} \quad (3.52)$$

Michelson observed an output similar to this when he used the red Balmer line in the spectrum of hydrogen at 6563 Å as the input to his interferometer and concluded that the line is actually a doublet (21), marking the first use of interferometric effects in spectroscopy. Since Michelson's detector was his eye he was able to observe only the envelop or *visibility curve* of the output intensity and thus was unable to fully analyze his spectra. Michelson devised an elaborately geared analog mechanism which could handle about 80 data points but did not use it extensively.

If the input is an idealized broadband source represented by  $B \text{ rect}(\bar{\nu}/2 \bar{\nu}_{\max})$  the interferogram is a sinc function:

$$C(x) = B \bar{\nu}_{\max} \text{ sinc}(2 \bar{\nu}_{\max} x) \quad (3.53)$$

The central lobe of this sinc function becomes narrower as  $\bar{\nu}_{\max}$  increases, approaching a delta function as  $\bar{\nu}_{\max} \rightarrow \infty$ . A realistic broadband source with gradually diminishing intensity also produces a highly localized interferogram that can be used to identify the  $x = 0$  or Zero Path Difference (ZPD) position in the interferogram.

For anything other than the simplest spectra, interpreting the untransformed intensity data is difficult or impossible. Figure 3.7 shows a  $0.01 \text{ cm}^{-1}$  resolution spectrum and the central part of the corresponding interferogram. Although Rubens and Wood calculated the first true spectra in 1911 (using a graphical trial and error technique), the need to perform a Fourier transform impeded the development of interferometric spectroscopy until the mid- 1960s, when the development Fast Fourier

Transform algorithms made the Fourier transform spectrometer a practical device by reducing the number of computations required to calculate a spectrum from  $O(N^2)$  to  $O(N \log_2 N)$ , where  $N$  is the number of data points (58). Today's and PC-based spectrometers can transform the interferograms into spectra almost instantaneously.

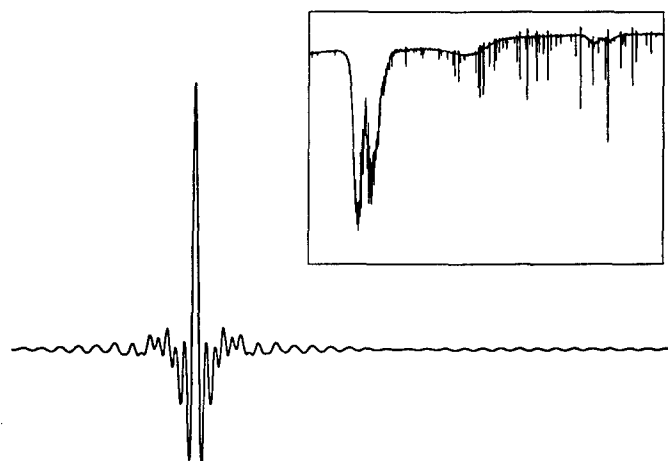


Figure 3.7 Central segment of an interferogram and the corresponding  $0.01 \text{ cm}^{-1}$  resolution spectrum.

**3.3.3 Limits on Resolution.** Equation (3.50) shows that if an exact representation of the spectrum is desired the interferogram must be determined for all positive retardations. Since the instrument is of finite extent, however,  $x$  may vary only over a finite range and the calculated spectrum is necessarily an approximation of the true spectrum. If the mirror moves a distance of  $\frac{1}{2} x_{\max}$  from ZPD so that  $x$  varies from 0 to  $x_{\max}$  this approximate spectrum is given by

$$B'(\bar{\nu}) = \int_0^{x_{\max}} C(x) \cos(2\pi\bar{\nu}x) dx. \quad (3.54)$$

This calculation is equivalent to finding the Fourier cosine transform of the ideal interferogram multiplied by the truncation function  $\text{rect}[x/(2x_{\text{max}})]$ . The transform of a product of two functions is the convolution of the transforms of the functions. The transform of the rect function is  $2 x_{\text{max}} \text{sinc}(2 x_{\text{max}} \bar{\nu})$ . If the input consists of one wavenumber component, we have, since the convolution of a delta function with any other function reproduces the other function,

$$\begin{aligned} B'(\bar{\nu}) &= 2 B(\bar{\nu}_0) x_{\text{max}} \text{sinc}[2(\bar{\nu}_0 - \bar{\nu})x_{\text{max}}] \\ &= 2 B(\bar{\nu}_0) x_{\text{max}} \frac{\sin[2\pi(\bar{\nu}_0 - \bar{\nu})x_{\text{max}}]}{2\pi(\bar{\nu}_0 - \bar{\nu})x_{\text{max}}} \end{aligned} \quad (3.55)$$

The effect of the finite scan length is to broaden the monochromatic source: the width at half max of the central lobe of the sinc function (Figure 3.8) is  $.605/x_{\text{max}} \text{ cm}^{-1}$  compared to the zero width of the input delta function. The approximate spectrum of two closely-separated monochromatic lines will be two over-lapping sinc functions and the lines may be so broadened that they cannot be resolved in the output spectrum.

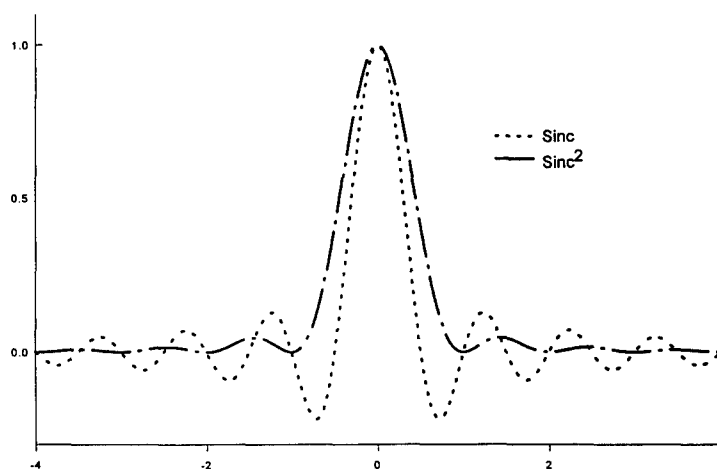


Figure 3.8 Normalized sinc and  $\text{sinc}^2$  spectra for same  $x_{\text{max}}$ .

The definition of resolution is somewhat arbitrary, but one criterion proposed by Lord Rayleigh states that two lines of equal intensity may be resolved when the peak of one falls at the first zero of the second. (Another criterion, that signal baseline be recorded between bands, is very stringent.) By this standard, the resolution of the approximate spectrum is  $.5/x_{\max}$   $\text{cm}^{-1}$ . In fact, two equal-intensity sinc spectra separated by this distance add to give one unresolvable maximum and the actual separation that allows two noiseless nearby lines to be barely resolved is approximately  $.66/x_{\max}$  (Figure 3.9). (This resolution criterion identifies minimum separation for which an intensity minimum exists between peaks.) Alternative resolution criteria may give a different number but the calculated resolution of the spectrometer is always proportional, at least to first order, to the reciprocal of the scan length.

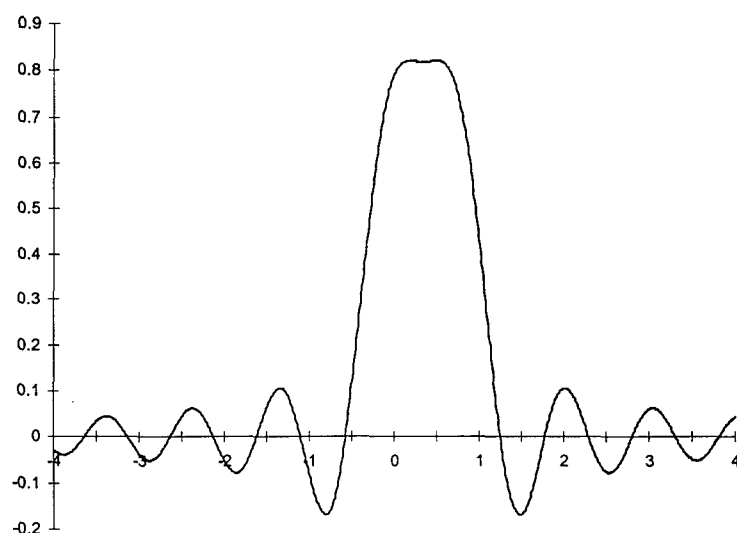


Figure 3.9 Two just-resolved sinc spectra. Separation is  $.67/x_{\max}$ .

The secondary positive and negative peaks of the sinc function that diminish in amplitude as the distance from the center of the function increases may cause a single narrow spectral line to become confused with the additional spectral features of a nearby line. The relative magnitudes of the secondary peaks are a function of

the truncation function that multiplies the ideal interferogram. If the truncation function converges slowly rather than abruptly to zero at  $x_{\max}$  the secondary oscillations will be greatly reduced. An unavoidable side effect of forcing the interferogram to converge slowly, however, is an increase in the relative width of the central peak and, consequently, a reduction of the resolution. The slow convergence of interferogram amplitudes is normally introduced computationally after an unattenuated finite interferogram has been recorded. This process is called *apodization*.

Boxcar apodization, equivalent to the rect function representing the effect of the finite scan length, gives the maximum resolution. The next simplest apodization function is the triangular function  $\text{tri}(x/x_{\max})$ , and its effect on the monochromatic spectrum can be found by convolving its transform,  $x_{\max} \text{sinc}^2(x_{\max} \bar{\nu})$ , with the idealized delta function spectrum. The magnitudes of the secondary lobes of the resulting  $\text{sinc}^2$  function (Figure 3.8) are less than those obtained without apodization but the line width is now  $.886/x_{\max} \text{ cm}^{-1}$ . (Note that the argument of the  $\text{sinc}^2$  function is half that of the sinc function for the same  $x_{\max}$ .) The resolution by the Rayleigh criterion is  $1/x_{\max}$  but in fact two noiseless lines separated by  $.84/x_{\max}$  can just barely be resolved (Figure 3.10).

The resolution of the spectrometer also depends on the size of the entrance aperture. The path lengths for light rays passing through different parts of the aperture are not equal. Although oblique rays travel farther than axial rays, they have a smaller path *difference* and the effective retardation of the spectrometer is smaller than that calculated assuming a perfectly collimated beam. The smaller effective retardation reduces the resolution of the instrument. An analysis of the effect shows that the resolution limit of the spectrometer is given approximately by

$$\Delta\bar{\nu} = \frac{\bar{\nu}_0 h^2}{8 F^2} \quad (3.56)$$

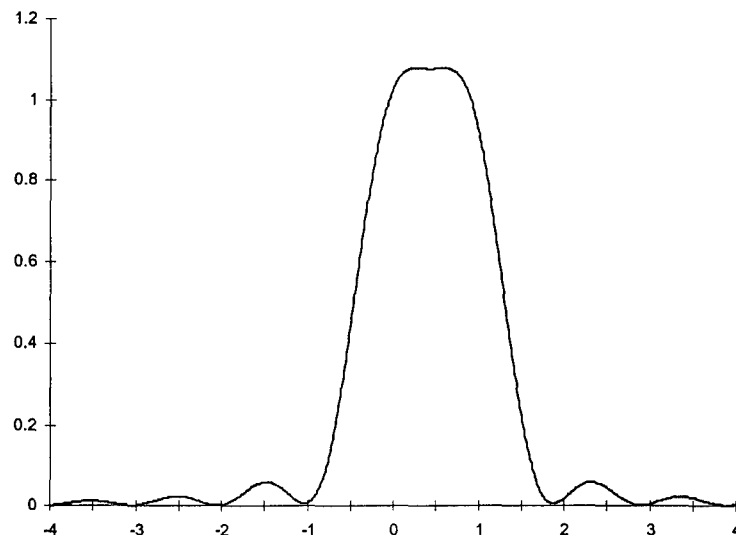


Figure 3.10 Two just-resolved  $\text{sinc}^2$  spectra. Separation is  $.84/x_{\text{max}}$ .

where  $\bar{\nu}_0$  is the wavenumber of the center of the spectrum,  $h$  is the diameter of the circular input aperture and  $F$  is the focal length of the collimator mirror (5). High resolution (smaller  $\Delta\bar{\nu}$ ) may therefore dictate a small aperture when spectra are obtained at high wavenumbers. Using an extended source also causes a shift in the location of the calculated spectral features but the effect is negligible.

The resolution of the spectrometer may be further reduced by poor alignment of the optical paths, by imperfections in its optical components, and by errors introduced when the analogue signal from the detector is amplified and digitized but these factors are minimized by proper design and operation. Modern interferometric infrared spectrometers are capable of resolutions less than the limits imposed by the sample effects described in Section 3.3.5.

**3.3.4 Bomem DA-8 FTIR Spectrometer.** The Bomem DA-8 FTIR spectrometer in our laboratory has a somewhat more complicated optical arrangement (Figures 3.11) and 3.12) than the basic interferometer described above. It uses a thermally-stabilized single-mode He-Ne laser to monitor the position of the moving mirror. The laser beam travels along the same path as the light from the source; a



window at the center of the beamsplitter transmits the laser light. The fixed mirror tilts around two axes to maintain system alignment as the moving mirror scans. The maximum mirror movement is 125 cm and the quoted maximum unapodized resolution is  $0.0026 \text{ cm}^{-1}$ . The smallest available aperture has a diameter of 0.5 mm which allows a maximum resolution of approximately  $.003 \text{ cm}^{-1}$  at  $4000 \text{ cm}^{-1}$  and  $0.005 \text{ cm}^{-1}$  at  $8000 \text{ cm}^{-1}$ . The next largest available aperture, with a diameter of 1.0 mm, allows a maximum resolution of  $0.011 \text{ cm}^{-1}$  at  $4000 \text{ cm}^{-1}$  and  $0.022 \text{ cm}^{-1}$  at  $8000 \text{ cm}^{-1}$ .

The intensity of the light transmitted through the sample is recorded at discrete points as the mirror scans at a constant speed. The sampling rate is automatically set to a value that prevents aliasing (58) and zero crossings of the reference laser are used to trigger intensity measurements at precisely known values of the mirror displacement. A dedicated vector processor performs a Fast Fourier Transform of the intensity data to calculate the spectrum.

A limited range of negative  $x$  values from  $-\Delta x$  to 0 is measured and used to verify that  $C(x)$  is an even function—in other words, that the interferogram is symmetric.

In order to co-add successive scans and obtain the spectrum via the Fourier transform algorithm it is necessary to locate a unique reference point, preferably close to the zero path difference (ZPD) position in the interferogram, that is highly repetitive from scan to scan. To this end, a secondary interferogram of a white light (broadband) source is used to produce a recognizable signal at the ZPD position. As described in Section 3.3.2, the white light is used because the broad, short wavelength radiation results in a very sharp, precise peak at ZPD, with virtually no other spectral features which might erroneously trigger a signal to collect data.

A folded-path gas cell like that developed by White (71) in 1942 increases the path length over which light from the source is absorbed by the sample, permitting the observation of weaker spectral features. The cell used in these experiments

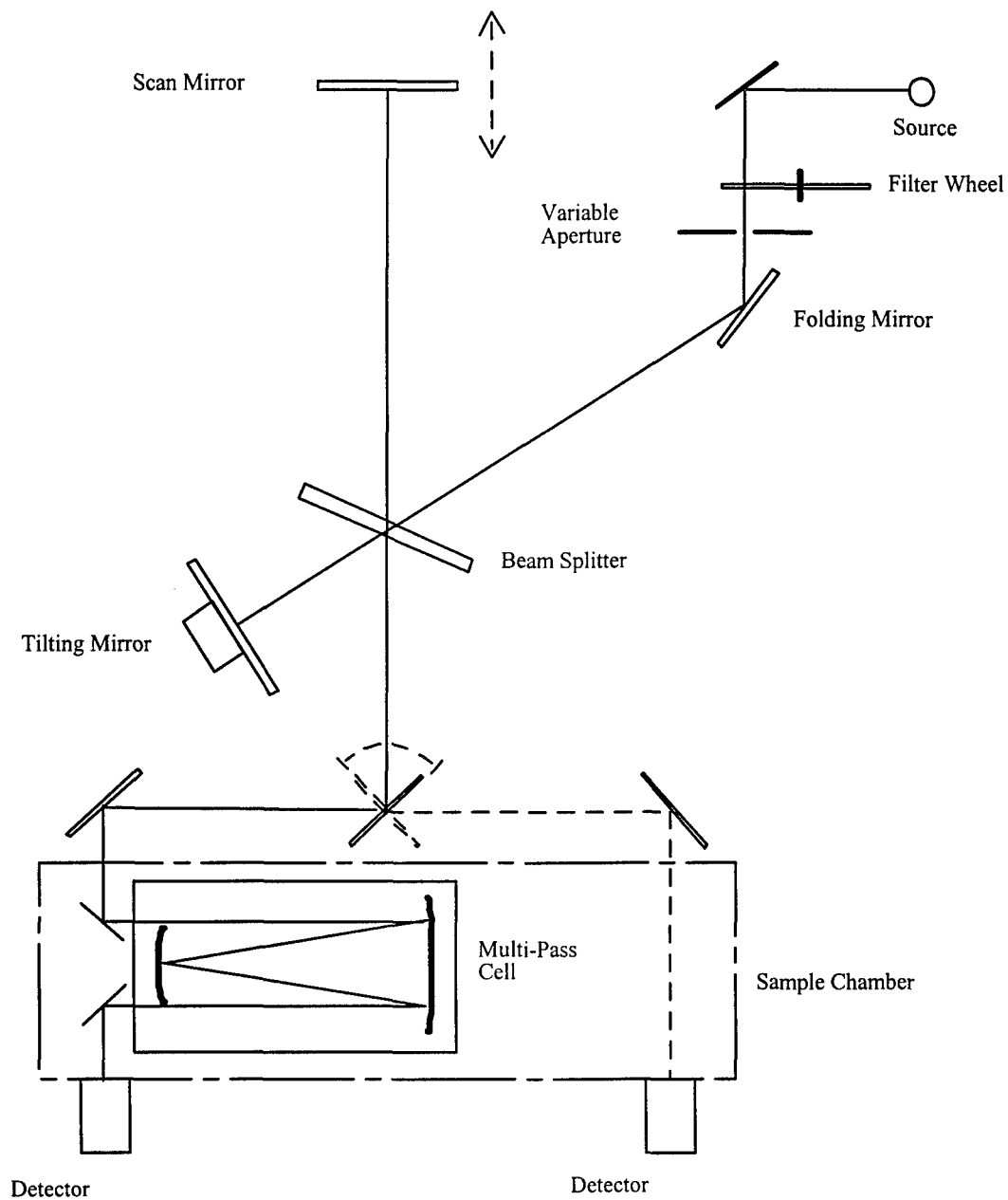


Figure 3.11 Schematic of Bomem DA-8 FTIR.

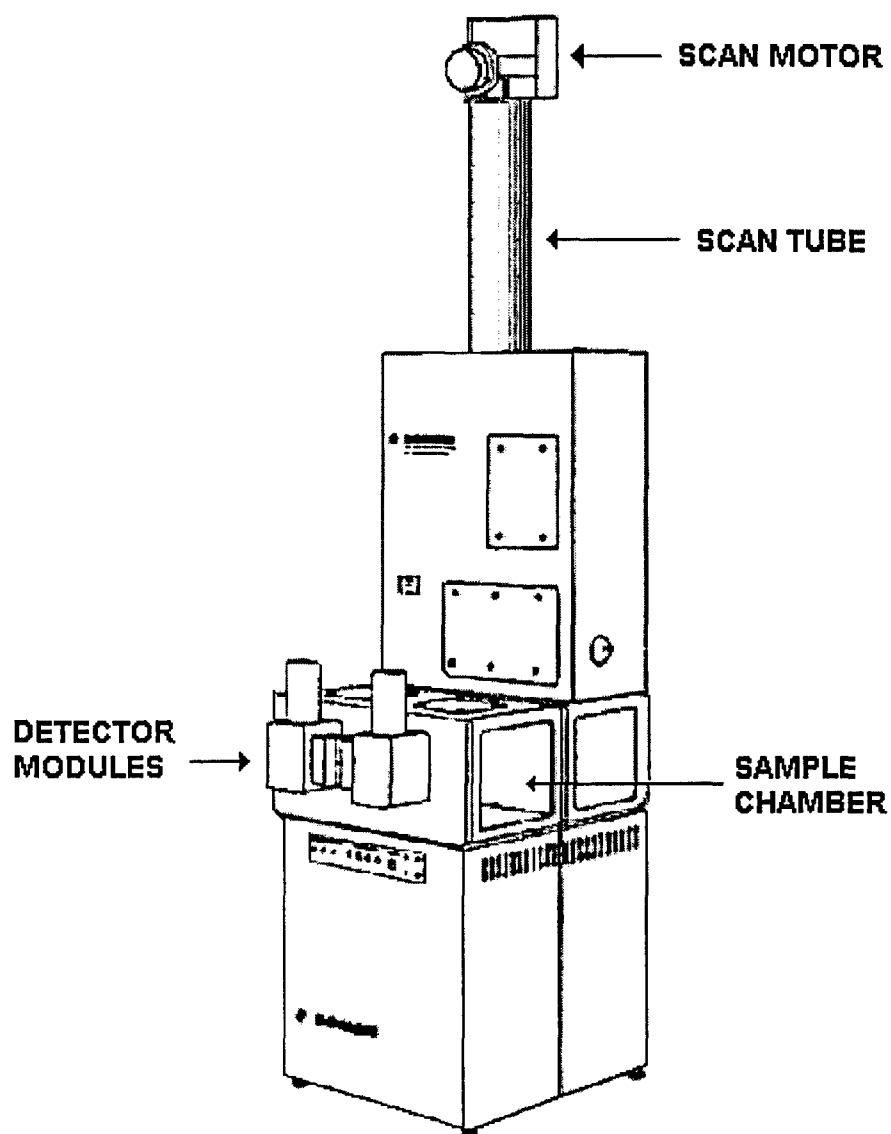


Figure 3.12 Bomem DA-8 Fourier Transform IR Spectrometer.

gives a total path length of 10 meters. Weak features may also be strengthened by increasing the pressure in the cell. The sample chamber along with the entire beam path can be evacuated to remove the effects of atmospheric absorbers such as water and carbon dioxide. Alternatively, a purge gas generator can be used to remove the water from the air before it flows through the spectrometer.

The sources are cooled by circulating water maintained at a set temperature by a chiller. In addition to preventing the sources from overheating, this minimizes intensity fluctuations that might complicate the addition of co-adds or the averaging of spectra.

The experimenter uses software running on a PC to select the source, set the diameter of the variable aperture, choose which filter is inserted in the beam path, determine which sample path is used, specify the resolution (maximum scan distance), set the scan speed (which varies with the detector response time), identify the detector and beam splitter being used, set the gain on the detector amplifier, and pick an apodization function. The FFT is performed by a vector processor which is part of a separate computer attached directly to the spectrometer.

The Bomem DA-8 spectrometer is easily adapted to such techniques as photo-acoustic spectroscopy, attenuated total reflectance, diffuse reflectance, etc. A wide variety of sources, beamsplitters and detectors enables operation from  $5\text{ cm}^{-1}$  to  $55000\text{ cm}^{-1}$ .

*3.3.5 Resolution and Accuracy of the Spectra.* For this experiment, the essential data are the positions of the ro-vibrational lines of BrNO. In order to determine these positions, it is first necessary to clearly distinguish the spectral lines from the noise that inevitably appears in the spectrum. The signal-to-noise ratio (SNR) of the spectra is therefore a paramount concern. The signal intensity can be optimized by selecting the combination of source, beamsplitter and detector that maximizes the observed response at the appropriate wavelengths without saturating

the detector or the A to D converters. Additionally, the mirror velocity can be chosen so that the temporal frequencies coincide with the best operating frequencies of the detector. If an appropriate band-pass filter is available, it can be used to reduce the total amount of light falling on the detector by narrowing the broad spectral output of the source to the specific region of interest. One advantage interferometric spectrometers have over dispersive devices is their larger throughput for a given resolution. This so-called Jacquinot or étendue advantage results from the optical difference between the two types of spectrometer. The resolution of a conventional grating-type spectrometer depends linearly on the instrument's slit width, and the detected power depends on the squares of the area of equal slits. Also, for high resolution, a spectrometer requires large radii for the collimation mirrors, and this condition in turn necessitates large  $f$ /numbers or small solid angles. An interferometer, on the other hand, can have a large circular source at the input with no strong limitation on resolution. Also, it can be operated with small  $f$ /numbers or with large solid angles at the source and detector. Consequently, more energy can be put through an interferometer than through a dispersive spectrometer.

The noise in IR detectors is essentially random and increases as the square root of the measurement time, while the signal increases proportionately to the measurement time. The SNR of a spectrum therefore tends to increase as the square root of the measurement time (or as the square root of the number of co-adds) and can be improved by taking more scans, either by averaging more co-adds per spectrum or by averaging separate spectra. The increase of the SNR with the square root of the number of scans is one manifestation of the Fellgett or multiplex advantage that arises because an interferometer receives information from the entire range of a given spectrum during each time element of a scan, whereas a conventional grating or prism spectrometer receives information only from the very narrow region which lies within the exit slit of the instrument. Fellgett's advantage can be used either to acquire spectra much faster or to improve the SNR for a given resolution, but is

often diminished in practice and may be lost entirely if the system is not detector-noise-limited.

Even if the spectrum has an adequate SNR, the spectral features cannot be identified if the spectral lines are so broad they blend together. In addition to the instrument-related factors discussed in Section 3.3.3, several sample-related mechanisms also affect the width of the lines.

Natural broadening, a function of the lifetime of the excited state, typically contributes no more than  $0.001 \text{ cm}^{-1}$  to the width of the line and is almost always negligible compared to other broadening mechanisms.

At low pressures ( $\leq 10$  torr) Doppler broadening is dominant and is given by (49)

$$\Delta \nu_D (\text{cm}^{-1}) = \frac{2\sqrt{2R \ln 2}}{c} \bar{\nu}_0 \sqrt{\frac{T}{M}} \quad (3.57)$$

where  $R$  is the gas constant, equal to  $8.314 \times 10^7 \text{ erg deg}^{-1} \text{ mol}^{-1}$ ,  $\bar{\nu}_0$  is the wavenumber of the center of the absorption line,  $T$  is the temperature in Kelvins and  $M$  is the atomic weight. For BrNO at 300K, using the average mass of the bromine isotopes, this works out to  $1.182 \times 10^{-6} \bar{\nu}_0$  wavenumbers, or approximately  $.004 \text{ cm}^{-1}$  at  $3500 \text{ cm}^{-1}$ . Doppler broadening produces a Gaussian line shape.

Pressure broadening becomes the dominant broadening mechanism at higher pressures. Lorentz broadening, caused by collisions between the absorbing gas molecules and foreign gas molecules, is proportional to the pressure of the foreign gas. Holtsmark broadening, due to collisions with atoms of the same kind, is a function of the oscillator strength and frequency of the absorption and is proportional to the concentration of the absorbing molecule. The lineshape of an absorption at frequency  $\nu_0$  due to Lorentz broadening is

$$S(\nu, \nu_0) = \frac{\nu}{\pi \nu_0} \left[ \frac{\Delta \nu}{(\nu_0 - \nu)^2 + (\Delta \nu)^2} + \frac{\Delta \nu}{(\nu_0 + \nu)^2 + (\Delta \nu)^2} \right] \quad (3.58)$$

Pressure broadening may therefore make a line asymmetrical as well as broadening it. If  $\Delta\nu \ll \nu$  and  $\nu \approx \nu_0$  the lineshape is symmetrical and is given by

$$S(\nu, \nu_0) = \frac{1}{\pi} \left[ \frac{\Delta\nu}{(\nu_0 - \nu)^2 + (\Delta\nu)^2} \right] \quad (3.59)$$

where  $\Delta\nu$  is now the half width at half height. Since  $\Delta\nu$  is inversely proportional to the time between collisions it is proportional to the density of the gas or, at fixed temperature, to the pressure. Pressure broadening is more difficult to predict than Doppler broadening but typically contributes approximately 0.0001 to 0.0004  $\text{cm}^{-1}$  per torr of total gas pressure at room temperature.

These lineshapes are convolved with the instrument line shape to give the observed line shape. Assuming that the various broadening sources are uncorrelated, the total broadening can be estimated as

$$\Delta\bar{\nu}_{\text{total}} = \sqrt{\Delta\bar{\nu}_{\text{inst}}^2 + \Delta\bar{\nu}_D^2 + \Delta\bar{\nu}_P^2}. \quad (3.60)$$

If the instrument resolution is 0.01  $\text{cm}^{-1}$  and the sample is 10 torr of BrNO at room temperature, the total broadening is less than 0.0115  $\text{cm}^{-1}$  at 3500  $\text{cm}^{-1}$ , only slightly more than the instrument resolution. If the sample pressure is increased to 40 torr, the total broadening is about 0.019  $\text{cm}^{-1}$ , or almost twice the instrument resolution.

While it is not practicable with our spectrometer to change the Doppler broadening by reducing the sample temperature, it is possible to vary the pressure of the sample gas and thereby change the pressure broadening. Although higher pressures lead to more broadening, they have the positive effect of making weak features more visible. It is necessary, therefore, to pick experimental configurations that are a compromise. The best way to quantify the various broadening mechanisms and pick the optimal experimental configuration is to compare spectra obtained at a variety of settings.

*3.3.6 Spectrometer Calibration.* The measurement of the positions of spectral lines is subject to both random and systematic errors. One source of systematic error is the air in the beam path—its index of refraction is a function of the observed wavelength and the humidity, pressure and temperature of the air. Systematic errors are corrected using high-resolution calibration standards such as  $\text{N}_2\text{O}$  and  $\text{H}_2\text{O}$ . Reporting the results in terms of these standards facilitates the comparison of data obtained in different laboratories.

The random error in the measured positions of the lines is largely determined by the resolution of the spectrum. Spectra taken at a lower instrument resolution have fewer data points per wavenumber interval. The peak of a line usually falls between data points; although interpolation of the data obtained with enough co-adds allows the error in the position of the line to be made less than the separation between data points, the positional accuracy is worse for lower resolutions. When observing weak spectral features at the highest resolutions, the many scans required to obtain an acceptable SNR combined with the increased time required for each scan (due to the longer scan length) can result in very long data acquisition times. It is therefore prudent to use the lowest resolution that allows the lines to be separated and identified. In order to obtain high positional accuracy, however, it may be necessary to use a higher resolution than that required to separate the lines. The reproducibility of the positions can be determined by comparing the peak positions from two or more spectra obtained at the same instrument resolution with all other factors affecting the resolution held constant. If the resolution of the calibration standards is much higher than that of the observed spectra, the dispersion in the observed positions of the calibration lines also provides a measurement of the experimental error. (See section 3.6.2).

Comparison of spectra with and without the sample in place allows the separation of instrument effects from real spectral features. A background scan taken with no sample in place can be used to convert the raw spectral data into a plot



of transmittance ( $I_{\text{sample}}/I_{\text{reference}} \times 100$ ) or absorbance ( $-\log I_{\text{sample}}/I_{\text{reference}}$ ) versus wavenumber. This is not necessary if one is interested only in the positions of the peaks but an uncorrected sloped background will bias the peak positions towards the higher baseline side.

### 3.4 Previous Work

Burns and Bernstein (10) obtained the first BrNO infrared spectra (400 to 5303  $\text{cm}^{-1}$  in 1950 and used the data to calculate force constants and amplitudes for the fundamental vibrational modes at 1801, 542 and 265  $\text{cm}^{-1}$ . Laane et al (41) improved on the work of Burns and Bernstein by analyzing the spectra of several isotopic species. This work studied the fundamental and combination vibrational bands of the three vibrations of nitrosyl bromide and concluded that  $\nu_1$  is due primarily to an NO bond stretch while  $\nu_2$  and  $\nu_3$  are largely mixes of an NBr stretch and an angle bending. The observed band centers are shown in Table 3.8. Laane was not able to resolve the infrared bands of  $^{79}\text{BrNO}$  and  $^{81}\text{BrNO}$ . The force constants (Table 3.9) were calculated using microwave data from an earlier study. This paper also discussed and tabulated the potential energy distribution, mean amplitudes, and inertial defect data for specific isotope combinations.

Degli Esposti *et al.* (13) analyzed high resolution ground vibrational level rotation spectra of the two isotopomers  $^{79}\text{BrNO}$  and  $^{81}\text{BrNO}$  and then used these results in an analysis of the  $v_1=0 \rightarrow v_1=1$  transition (12). They determined the rotational constants for these transitions and used this information to determine the cubic force constants. In their study of the  $\nu_1$  transition, this group prepared nitrosyl bromide by mixing NO and gaseous bromine at room temperature in a 20 cm long glass cell equipped with calcium fluoride ( $\text{CaF}_2$ ) windows. The spectrum of the 1.5 torr sample was recorded with a Bruker IFS 120HR Fourier transform spectrometer at .0045  $\text{cm}^{-1}$  resolution using a globar source, a potassium bromide (KBr) beamsplitter, and a mercury cadmium telluride (MCT) detector. This group calibrated the positions of

Table 3.8 Band centers ( $\text{cm}^{-1}$ ) of BrNO for isotopes of N and O.

	$^{16}\text{O}^{14}\text{NBr}$	$^{16}\text{O}^{15}\text{NBr}$	$^{18}\text{O}^{14}\text{NBr}$	$^{18}\text{O}^{15}\text{NBr}$	Relative Intensity
$\nu_1$	1799.0	1768.3	1751.5	1719.5	VVVS
$\nu_2$	542.0	527.8	No Data	521.5	VS
$\nu_3$	266.2	264	No Data	257.0	S
$\nu_2 + \nu_3$	807.2	791	No Data	777.5	M
$2\nu_2$	1078	No Data	No Data	No Data	VW
$\nu_1 - \nu_2$	1256	No Data	No Data	No Data	VW
$\nu_1 - \nu_3$	1531	No Data	No Data	1463	VW
$3\nu_2$	1605	No Data	No Data	No Data	VW
$\nu_1 + \nu_3$	2065.2	2032.6	2009	1976.0	M
$\nu_1 + \nu_2$	2341.6	2297.6	No Data	2242.2	MW
$\nu_1 + 2\nu_2$	2878.2	2820	No Data	2760.0	VW
$2\nu_1$	3562.1	3503.1	3470.9	3408.1	S
$2\nu_1 + \nu_3$	3827.7	3766.5	No Data	3665.1	MW
$2\nu_1 + \nu_2$	4107.2	4033	No Data	3928.6	W
$3\nu_1$	5296	5206	5158	5066	MW
$3\nu_1 + \nu_3$	5562	No Data	No Data	5324	VW
$3\nu_1 + \nu_2$	5841	5740	No Data	5591	VVW
$4\nu_1$	6994	6878	No Data	6695	VW

the BrNO absorption lines using residual water absorption lines. They observed only a-type transitions ( $\Delta K_a = 0$ ) for rotational levels up to  $J = 70$  and  $K_a = 10$  in the dominant P and R branches and identified a weaker Q branch feature on the shoulder of the P branch. The band origins, rotational constants and other parameters for  $^{79}\text{BrNO}$  and  $^{81}\text{BrNO}$  reported by Degli Esposti appear in Table 3.10.

### 3.5 Experimental

**3.5.1 Experimental Procedures.** Bromine and NO were purified using the procedures described in Chapter II, then mixed by putting bromine in the cell and then adding NO until the desired final pressure was achieved. Most of the spectra were obtained using a multi-pass cell (total path length 10 meters) fitted with KBr input/output windows but a single-pass cell 20 cm long with  $\text{CaF}_2$  windows was used for recording the strong  $\nu_1$  spectrum. Some scans were taken using isotopically-

Table 3.9 Force constants of BrNO.

	Calculated Value
$F_{\text{NO}}$	$15.25 \pm 0.04 \text{ md/\AA}$
$F_{\text{NBr}}$	$1.13 \pm 0.05 \text{ md/\AA}$
$F_{\alpha}$	$1.13 \pm 0.02 \text{ md \AA/rad}^2$
$F_{\text{NO,NBr}}$	$1.47 \pm 0.36 \text{ md/\AA}$
$F_{\text{NO},\alpha}$	$0.11 \pm 0.20 \text{ md/rad}$
$F_{\text{NBr},\alpha}$	$0.10 \pm 0.02 \text{ md/rad}$

enriched bromine (90%  $^{81}\text{Br}$ /10%  $^{79}\text{Br}$ ) obtained from ICON for comparison with the scans of BrNO made with non-enriched bromine (49.46%  $^{81}\text{Br}$ /50.54%  $^{79}\text{Br}$ ) in order to distinguish the spectral features of the two isotopomers. (The natural isotopic abundances of oxygen and nitrogen are 99.63%  $^{14}\text{N}$  and 99.759%  $^{16}\text{O}$ ; the observable spectra are due entirely to molecules composed of these isotopes.) Since only a small amount of the isotopically-enhanced bromine was available it was not purified prior to use to avoid any loss. The widely-spread BrNO spectra were obtained using either a globar or a quartz halogen source with a KBr or  $\text{CaF}_2$  beamsplitter and an InSb or MCT detector. The source spectrum was narrowed using a band-pass filter when the appropriate filter was available.

The spectra were obtained using the highest practical resolution, usually  $0.005 \text{ cm}^{-1}$  but dropping to  $0.01 \text{ cm}^{-1}$  for the weaker bands. Figure 3.13 shows the impact of using the lower resolution. Analysis of the spectra obtained in this and previous efforts indicated that a resolution of  $0.005 \text{ cm}^{-1}$  allows most of the lines in the spectra to be identified and their positions determined. When necessary a resolution of  $0.01 \text{ cm}^{-1}$  was used—even this resolution necessitated the use of the smallest available aperture for those spectra found above  $4000 \text{ cm}^{-1}$ ; the resulting reduced signal mandated many more scans in this region. Low pressures ( $\leq 10 \text{ torr}$ ) made the pressure broadening negligible; Doppler broadening made the actual resolution of a spectrum taken at  $0.005 \text{ cm}^{-1}$  instrument resolution about  $.0064 \text{ cm}^{-1}$ .

Table 3.10 Molecular constants of the  $\nu_1$  fundamental band for two isotopomers of BrNO. (Band origins in  $\text{cm}^{-1}$ , rotational constants in MHz. The asymmetry parameter  $\kappa$  is dimensionless. Standard errors in units of the last quoted digit are in parentheses for the fitted constants. \*Both levels share common value.)

	$^{79}\text{BrNO}$		$^{81}\text{BrNO}$	
	$v_1 = 0$	$v_1 = 1$	$v_1 = 0$	$v_1 = 1$
$\nu_0$	1798.751285(53)		1798.742722(57)	
A	85500.4620(99)	84720.73(11)	85482.944(12)	84703.09(11)
B	3747.07053(22)	3762.6039(44)	3722.34778(27)	3737.8017(47)
C	3585.98785(24)	3598.9833(39)	3563.30894(30)	3576.2520(43)
$\kappa$	-0.996067052	-0.9959660	-0.99611720	-0.9960174
$\Delta_J (10^{-3})$	2.852185(88)	2.88560(37)	2.816479(78)	2.84996(39)
$\Delta_{JK} (10^{-2})$	-5.69179(43)	-5.6952(27)	-5.66109(45)	-5.6676(31)
$\Delta_K$	4.82550(50)	4.7272(12)	4.80520(76)	4.7096(13)
$\delta_J (10^{-4})$	1.57887(22)	1.6145(47)	1.54934(11)	1.5881(51)
$\delta_K (10^{-2})^*$	1.9859(83)		1.938(12)	
$\Phi_J (10^{-10})^*$	4.068(13)		4.068	
$\Phi_{JK} (10^{-7})^*$	1.2012(65)		1.1179(17)	
$\Phi_{KJ} (10^{-5})^*$	-2.9615(32)		-2.9315(27)	
$\Phi_K (10^{-10})^*$	2.149(58)		2.149	

Individual spectra were compared to wavelength standards before being averaged to correct small variations between the systematic line position shifts present in each spectrum. Each averaged spectrum was weighted according to the number of co-adds used to obtain it so that spectra obtained with fewer co-adds were not over-represented in the average.

*3.5.2 Analysis Techniques.* Once a calibrated, high-quality spectrum is obtained, the BrNO lines must be identified. The positions of the BrNO lines are determined from the position of their peaks and by finding the center of the lines. Any asymmetry in a line was assumed to be caused by the blending of one or more nearby lines and not by pressure broadening or other mechanisms. The centers of closely spaced blended lines were determined by fitting the spectra to selected line

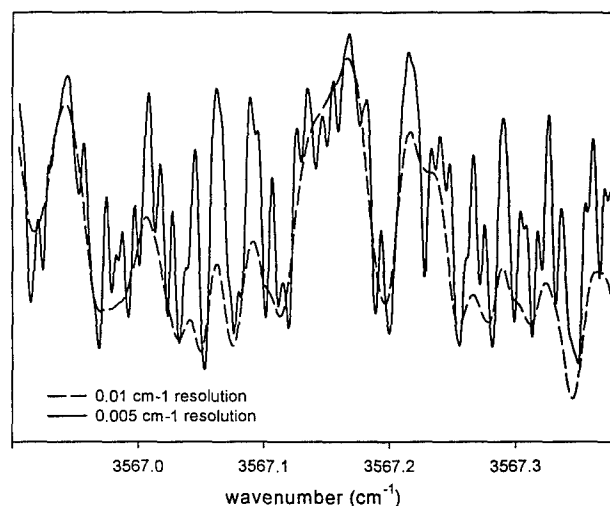


Figure 3.13 Two spectra taken at resolutions of  $0.01 \text{ cm}^{-1}$  and  $0.005 \text{ cm}^{-1}$ .

shapes. Since the number, height and shape of the blended lines are not known exactly the error in the deduced positions of the blended lines is inevitably larger than that of unblended lines. Figure 3.14 shows a number of spectral features and six gaussian lines that fit them reasonably well. These gaussian lines were selected by trial and error. Although software to fit selected line shapes to spectra is available, the large number of lines in the BrNO spectra made it more practicable to estimate the positions of blended lines.

After the locations of the BrNO absorption lines are determined, the lines must be assigned to specific energy level transitions. The large number of transitions and the absence of easily identifiable patterns makes this the hardest part of the analysis, but the line positions and strengths given by the symmetric top approximation are useful guides, as are the results of previous studies.

Once the spectrum is assigned, the Hamiltonian is solved numerically and its parameters varied to give the best fit to the observed lines and their assignments. This process is repeated until the differences between the predicted and observed line positions are no larger than the estimated experimental error in the line positions.

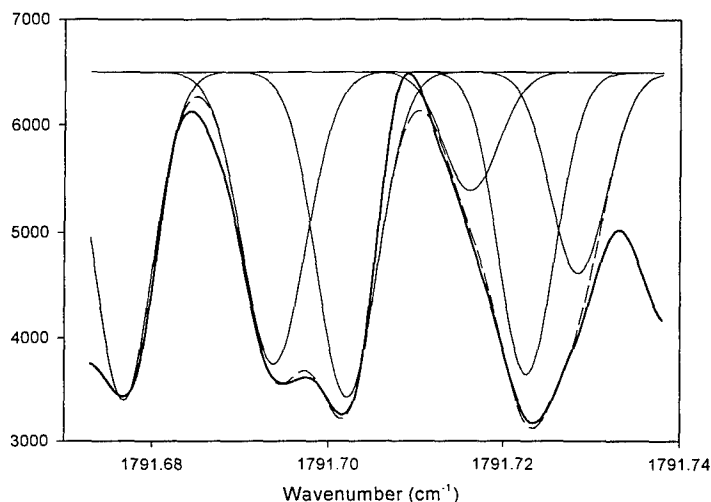


Figure 3.14 Six gaussian lines chosen to fit spectrum.

Blended lines are given less weight in the fit or, if ambiguous, used as a check on the assignment and parameter fit which, if correct, will give the positions of the blended lines not included in the fit.

A Fortran computer program (Appendix A) written by Matt Elrod and obtained from C. Degli Esposti (Dept of Chemistry, University Degli Studi di Bologna) was used to fit the Hamiltonian constants to the observed line positions. The computer program diagonalizes the Hamiltonian matrix discussed in Section 3.2.3 and then minimizes the nondimensional quantity

$$\chi^2 = \sum_{i=1}^N \left( \frac{y_i - y(x_i; a_1 \dots a_M)}{\sigma_i} \right)^2 \quad (3.61)$$

where  $y_i$  is the measured position of spectral line  $i$ ,  $N$  is the number of observed lines,  $y(x_i; a_1 \dots a_M)$  is the position of line  $i$  predicted using the energy levels resulting from the diagonalization of the Hamiltonian matrix and  $\sigma_i$  is the error in the measurement of the line position. The predicted line positions are a function of  $x_i$  (the  $J$ ,  $K_a$  and  $K_c$  values that identify the upper and lower energy levels) and  $a_1 \dots a_M$ , the parameters in the Hamiltonian. The program performs the nonlinear fit using a singular value

decomposition (SVD) routine incorporating the *Levenberg-Marquardt method* (58). For an overdetermined system (number of observations larger than number of fitted parameters), this fitting routine produces a solution that is the best approximation in the least-squares sense. The program lists the difference between the observed and predicted line positions and provides other data required to judge the goodness of the fit, including the final  $\chi^2$  value and the correlation matrix. The fitting routine can be bypassed and the program used to predict line positions but it provides no information on the intensity of the absorption lines.

### 3.6 Results

*3.6.1 Validation of Fitting Program.* The fitting program was validated using several techniques. The first consisted of using the program to predict a set of lines based on a representative set of rotational constants, then adding random errors to the predicted line positions and using the program to fit the band origin and upper level rotational parameters to the randomly shifted line positions. This validation technique demonstrates that the fitting routine incorporated into the program works correctly and also demonstrates the relationship between the errors in the input positions and the statistics of the fit.

Figures 3.15 and 3.17 are plots of the random errors between  $\pm .001 \text{ cm}^{-1}$  and  $\pm .01 \text{ cm}^{-1}$  added to the positions of 496 lines. Figures 3.16 and 3.18 show that the fitting procedure predicts the line positions with the same uncertainty. Table 3.11 compares the parameters used to determine the line positions before the errors were introduced with the fitted parameters and gives the values of  $\chi^2$  reported by the program. The input parameters are within the error bounds of the fitted parameters and the values of  $\chi^2$  properly reflect the quality of the fits. (A rule of thumb (58) is that a "typical" value of  $\chi^2$  for a "moderately" good fit is  $\chi^2 \approx N - M$ , where  $N$  is the number of observations and  $M$  the number of fitted parameters. Equation 3.61 on page 3-53 defines  $\chi^2$ .) The last column of Figure 3.11 shows that adding a constant

$0.02 \text{ cm}^{-1}$  offset to the  $\pm .01 \text{ cm}^{-1}$  errors shifts the position of the band origin by  $0.01988 \text{ cm}^{-1}$ ; the rotational constants are essentially unchanged. This is expected because the band origin contributes an additive constant to the line positions.

A similar analysis including the distortion constants showed that the sextet constants are difficult to fit accurately when errors are introduced, especially when high J terms are omitted. The effect of the sextet terms becomes more pronounced as J and K increase, but the lines get weaker and become difficult to identify unambiguously and locate accurately. For these reasons the sextet constants were held fixed to their ground state values (12).

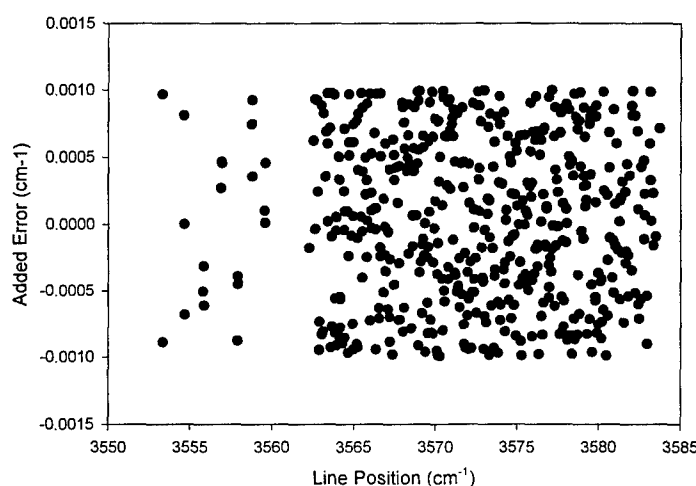


Figure 3.15 Random  $\pm .01 \text{ cm}^{-1}$  errors added to line positions predicted using parameters listed in Table 3.11.

The program was also checked by comparing its output with the approximate positions of the lines given by the symmetric top approximation (Section 3.2.7). Figure 3.19 shows the difference between the line positions given by the approximation and by diagonalization for some R branch transitions. No distortion terms were included in either calculation. Figure 3.20 shows the difference for  $J \leq 30$ . Figure 3.21 shows the error in the second differences. As expected, the difference



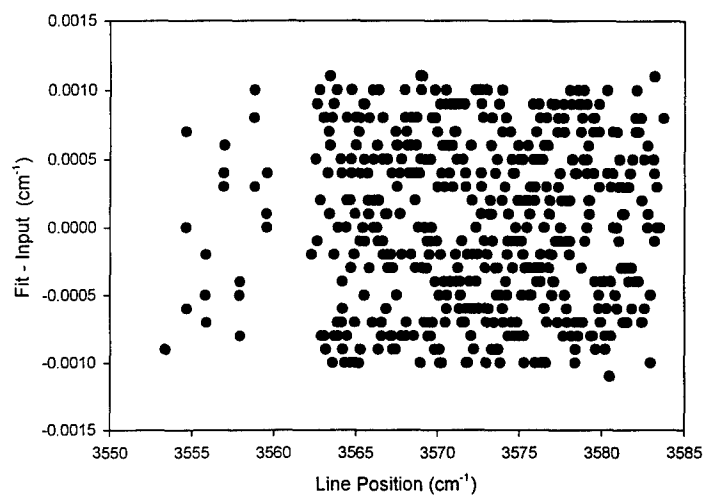


Figure 3.16 Difference between input positions and fit results after random  $\pm .01 \text{ cm}^{-1}$  errors shown in Figure 3.15 were added to predicted line positions.

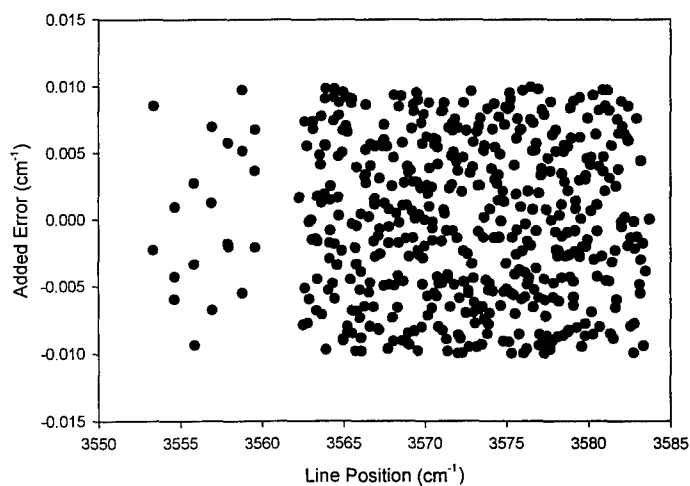


Figure 3.17 Random  $\pm .001 \text{ cm}^{-1}$  errors added to line positions predicted using parameters listed in Table 3.11.

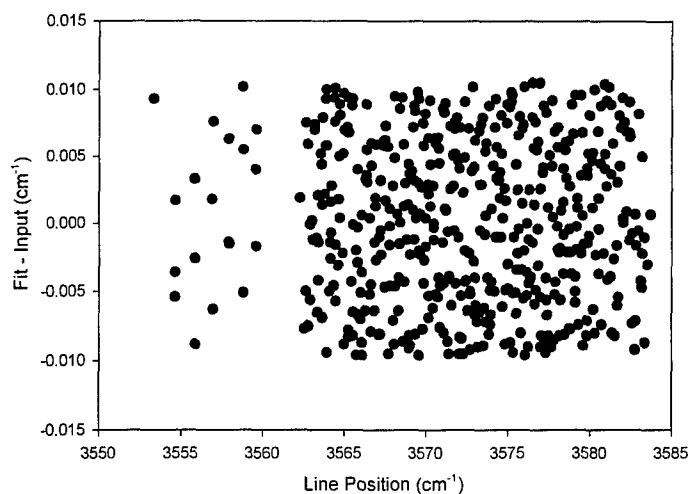


Figure 3.18 Difference between input positions and fit results after random  $\pm .001 \text{ cm}^{-1}$  errors shown in Figure 3.17 were added to predicted line positions.

between the program's results and approximation is larger at higher  $J$  but decreases as  $K$  increases (Section 3.2.2).

*3.6.2 Spectrometer Calibration.* Although the index of refraction of the air in the spectrometer is a function of temperature and humidity, which were only loosely controlled, comparison of calibration spectra taken at different times indicated that these factors made only insignificant contributions to the wavenumber shift required to calibrate the spectrometer.

Water is an excellent calibration standard but its presence in the spectrometer may mask other features. Background spectra taken with no BrNO in the cell are used to identify contaminant lines. Figure 3.22 shows two spectra, one of water only and one of BrNO with water contamination. The water lines are broader than the BrNO lines because  $\text{H}_2\text{O}$  is more Doppler-broadened.

Since the uncertainty in the calibration standards (23) is very small, the dispersion in the line positions is almost entirely a measure of the error in the observations.

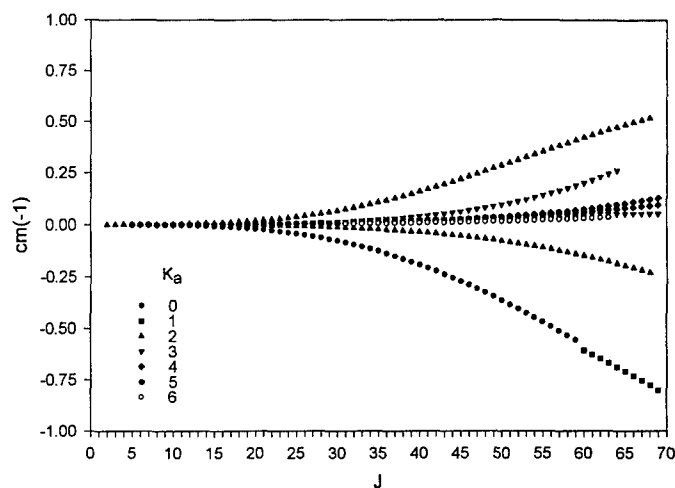


Figure 3.19 Difference between line positions given by diagonalization and by symmetric top approximation.  $\Delta J = 1$ ,  $\Delta K_a = 1$ .

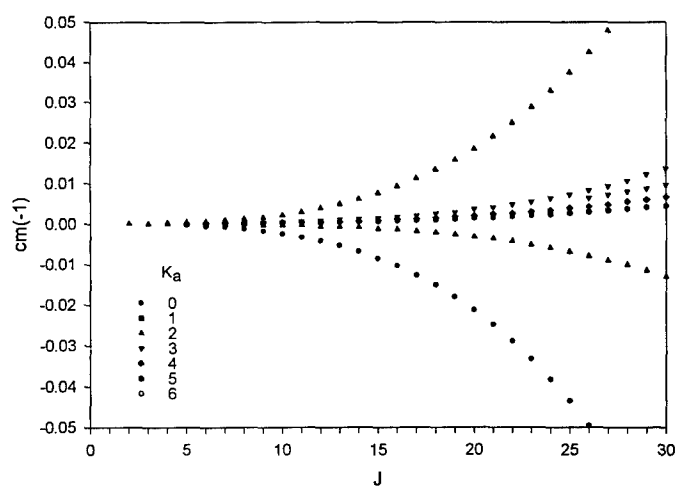


Figure 3.20 Difference between line positions given by diagonalization and by symmetric top approximation.  $\Delta J = 1$ ,  $\Delta K_a = 1$ .

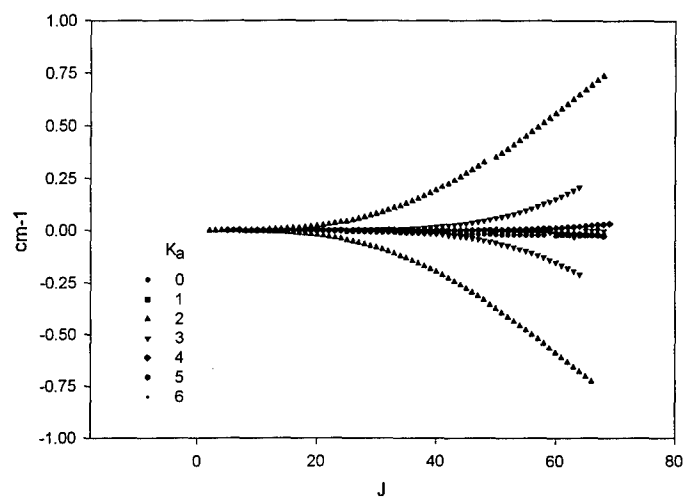


Figure 3.21 Error in second differences calculated using symmetric top approximation.  $\Delta J = 1$ ,  $\Delta K_a = 1$ .

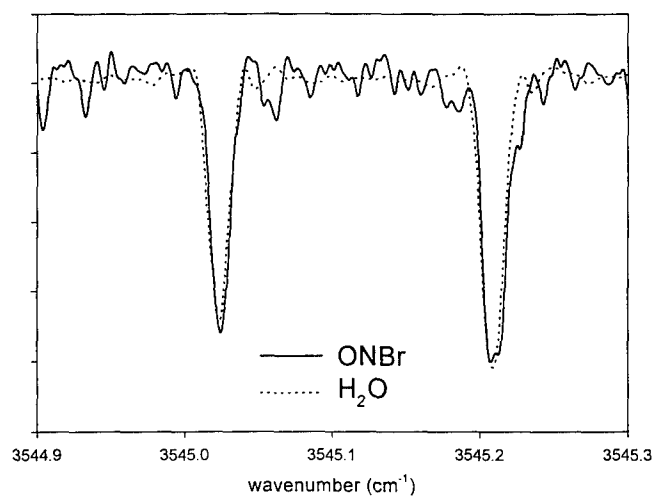


Figure 3.22 Water in BrNO spectrum.

Table 3.11 Comparison of predicted and input parameters with known errors. All parameters except iterations in MHz.

	INPUT	$\pm .001 \text{ cm}^{-1}$ FIT	$\pm .01 \text{ cm}^{-1}$ FIT	$\pm .01 \text{ cm}^{-1} + .02 \text{ cm}^{-1}$ FIT
A	839240.00	$83940.00 \pm .04$	$83939.90 \pm .40$	$83939.89 \pm .3944$
B	3778.08	$3778.08 \pm .001$	$3778.08 \pm .01$	$3778.08 \pm .01347$
C	3611.99	$3611.99 \pm .001$	$3611.99 \pm .01$	$3611.98 \pm .01$
$\nu_0$	106789071	$106789071 \pm 1.534$	$106789067 \pm 14.90$	$106789663 \pm 14.90$
$\chi^2$		327.99	30928.78	31001.52
iterations		10	10	10

The calibration plots show that the uncertainty in the positions of the lines is approximately one tenth of the resolution of the spectrum. (Figure 3.23 used less accurate calibration standards (11) and the dispersion reflects both sources of error.) Figures 3.23-3.26 are based on scans taken with the  $\text{CaF}_2$  beamsplitter, InSb detector and quartz source.

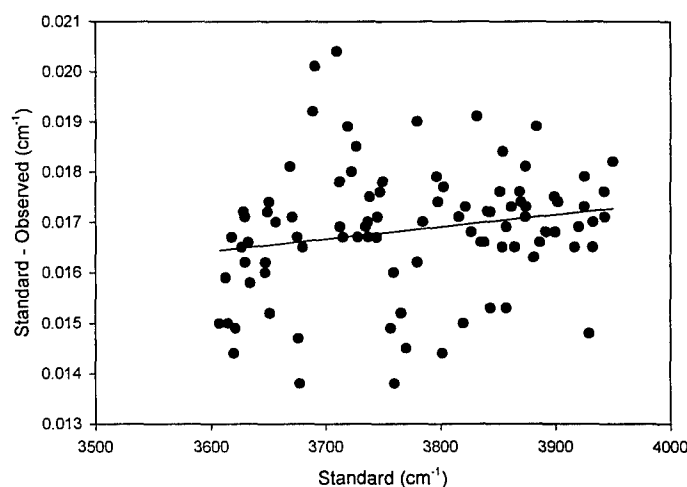


Figure 3.23  $\text{H}_2\text{O}$  Calibration. Resolution of Observed Lines  $0.01 \text{ cm}^{-1}$ . Error in standard lines  $\pm 0.001 \text{ cm}^{-1}$ .

The four calibrations are shown together in Figure 3.27. The data support only a linear fit over this range; the shift required to calibrate the spectrometer is

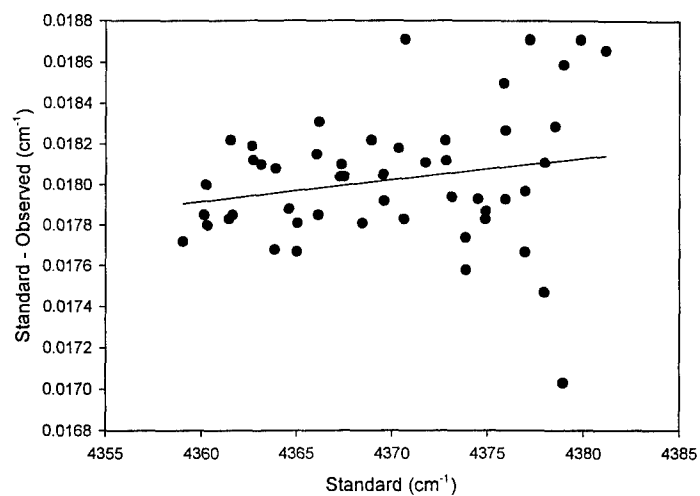


Figure 3.24  $\text{N}_2\text{O}$  Calibration. Resolution of Observed Lines  $0.004 \text{ cm}^{-1}$ . Error in standard lines  $\pm 0.00003 \text{ cm}^{-1}$ .

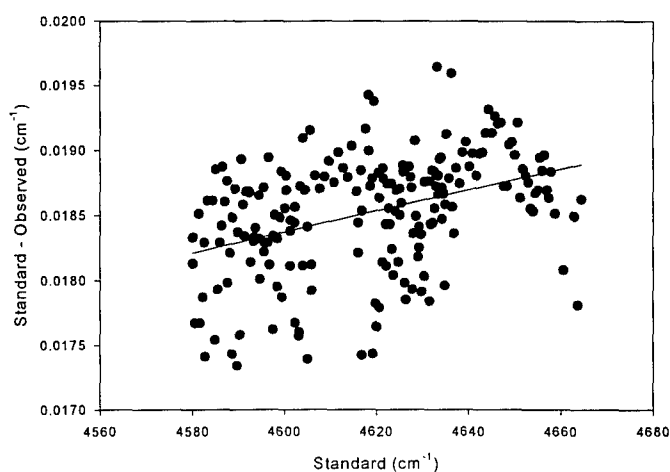


Figure 3.25  $\text{N}_2\text{O}$  Calibration. Resolution of Observed Lines  $0.007 \text{ cm}^{-1}$ . Error in standard standard lines  $\pm 0.00003 \text{ cm}^{-1}$ .

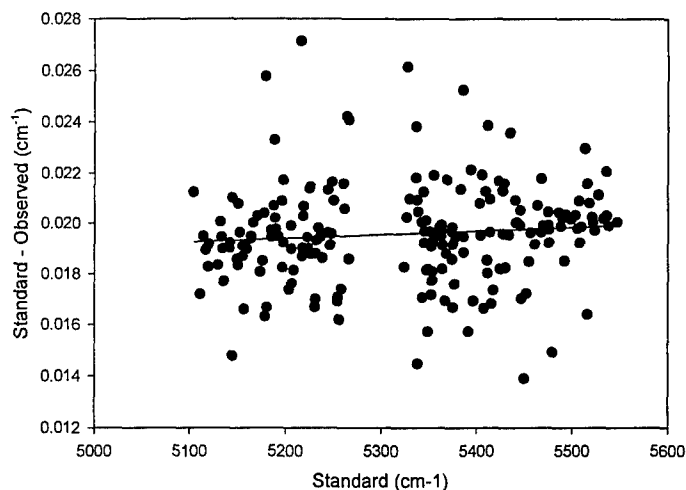


Figure 3.26 H<sub>2</sub>O Calibration. Resolution of Observed Lines 0.02 cm<sup>-1</sup>. Error in standard lines  $\pm 0.00003$  cm<sup>-1</sup>.

$0.010357 + 1.74575 \times 10^{-6} \bar{\lambda}$ . Over a 200 cm<sup>-1</sup> wide BrNO band the required shift varies by 0.000349 cm<sup>-1</sup>, or a little less than the accuracy of the line positions when the resolution is 0.005 cm<sup>-1</sup>. In Figure 3.28 the baseline noise for a typical 0.01 cm<sup>-1</sup> spectrum is plotted to the same scale as part of the BrNO absorption from the same spectrum over a width of .2 cm<sup>-1</sup>. (The baseline was shifted from the wings of the spectrum.) This spectrum, the average of 300 co-adds taken with an InSb detector, a CaF<sub>2</sub> beamsplitter and a quartz halogen source, has an RMS noise level of about  $\pm 17$  arbitrary absorption units about the baseline at 2128 units. The absorption lines in this part of the spectrum near 1515 cm<sup>-1</sup> bottom out at about 540 units giving a signal level of 1588 units and an SNR of 45.

*3.6.3 Spectra.* Figure 3.29 is a composite of two low resolution scan showing most of the spectra considered in this study.

Spectra of the BrNO bands observed during this study are shown below, plotted as transmittance versus wavenumber. (Not all of these spectra were analyzed.) The pressure in the cell was not the same for all the plotted spectra so the transmittances

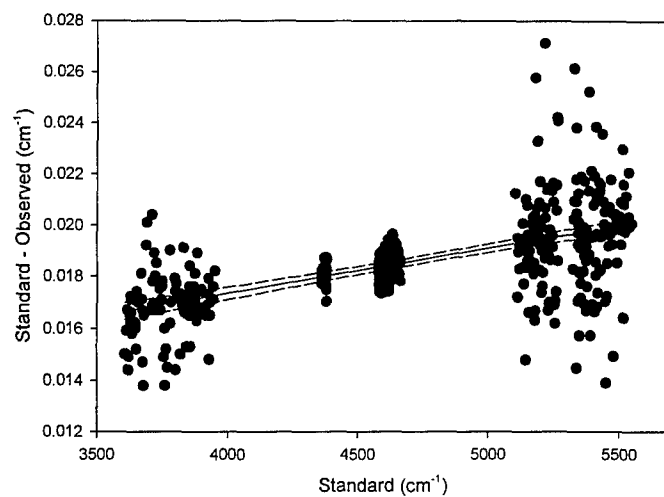


Figure 3.27 Spectrometer calibrations with linear least squares fit and 99% confidence intervals.

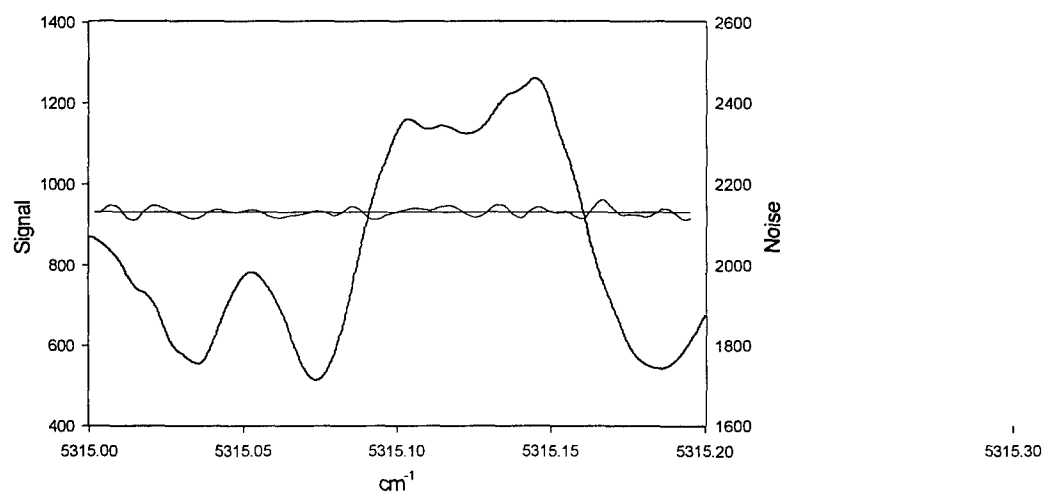


Figure 3.28 Comparison of signal and baseline noise level for 0.01 cm⁻¹ resolution spectrum (300 co-adds).



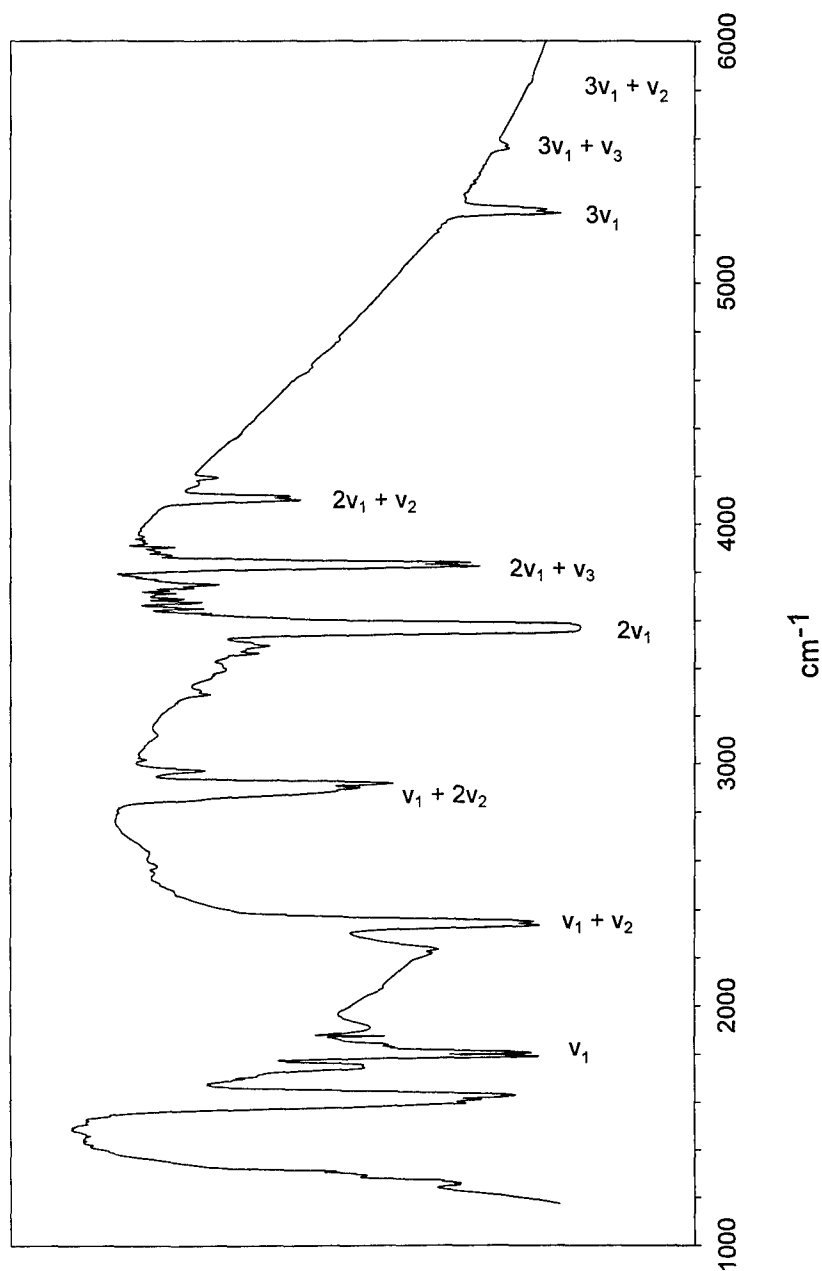


Figure 3.29 Overview of BrNO absorption spectra.

cannot be compared directly. The abnormally deep absorption lines in some of the spectra are due to  $\text{H}_2\text{O}$  contamination. Despite repeated efforts, including heating the cell and pumping on it for extended periods, the water vapor lines could not be eliminated. The water lines are easy to identify, however, and only when the water vapor lines were intense enough to saturate the absorption did they prevent the identification of the underlying  $\text{BrNO}$  lines.

The  $2\nu_1$  spectrum shown in Figure 3.30 shows the features common to the spectra of non-overlapping bands. The P and R branches are easily identified. The dense structure of the spectrum is illustrated in Figure 3.31, which shows a one wavenumber wide section of the P branch at  $0.005\text{ cm}^{-1}$  resolution. Part of the Q branch is shown in Figure 3.32 at  $0.01\text{ cm}^{-1}$  resolution.

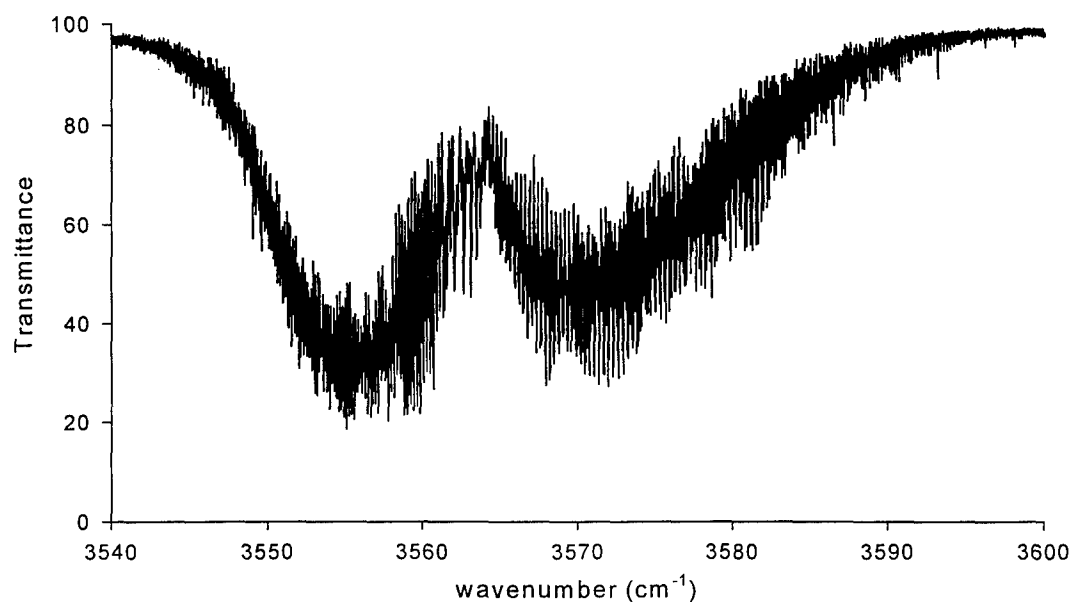


Figure 3.30 Spectrum of  $2\nu_1$  band of  $\text{BrNO}$ .

The  $\nu_1 + \nu_2$  and  $\nu_1 + 2\nu_3$  bands, shown in Figure 3.35, and the  $2\nu_1 + \nu_2$  and  $2\nu_1 + 2\nu_3$  bands, shown in Figure 3.38, are due to transitions that terminate on the  $(2\ 1\ 0)$  and  $(2\ 0\ 2)$  levels which are separated by about  $10\text{ cm}^{-1}$ . When the energies of two vibrational levels with the same symmetry are within approximately  $10\text{ cm}^{-1}$

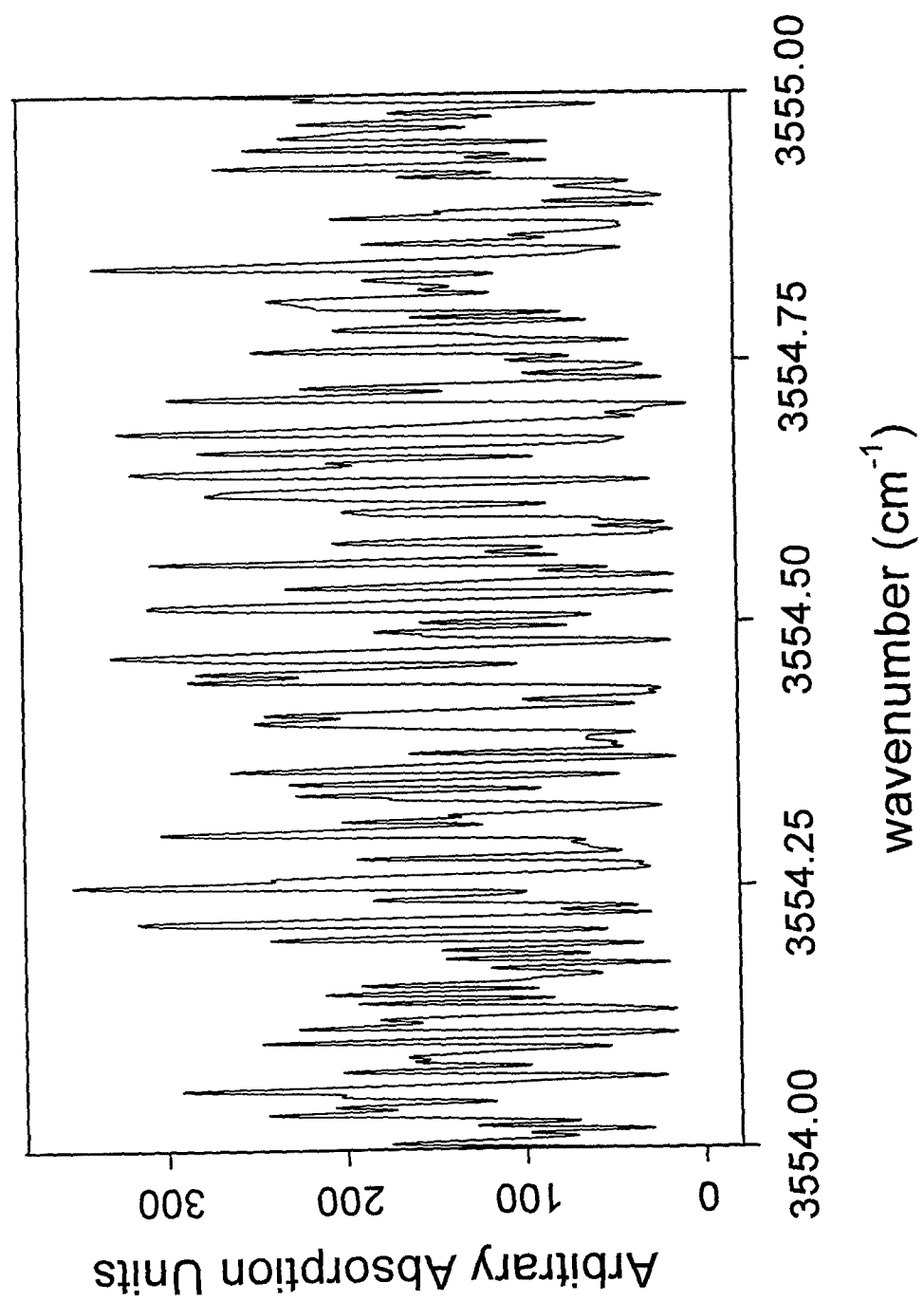


Figure 3.31 A segment of the  $2\nu_1$  P branch spectrum.

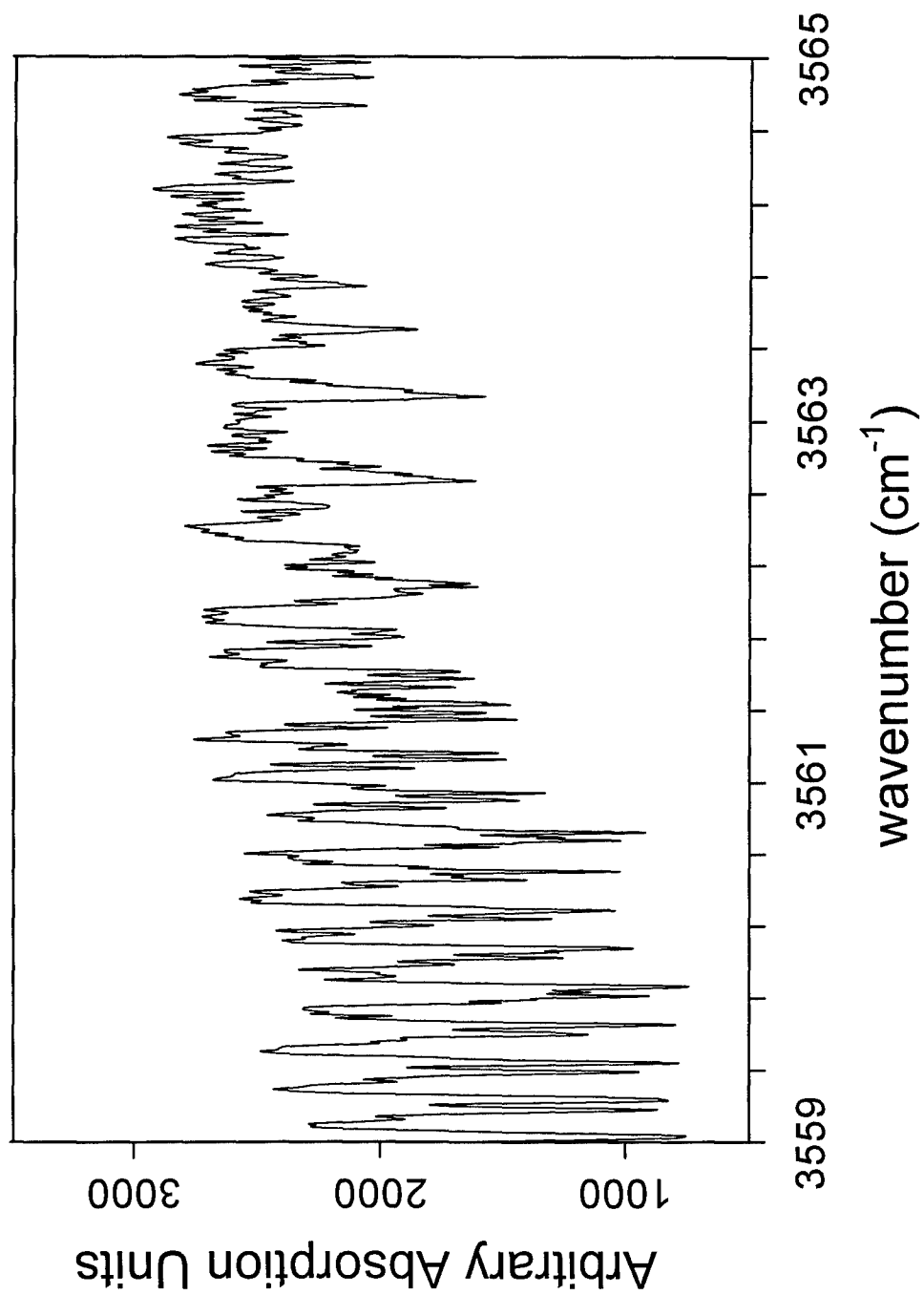


Figure 3.32 A portion of the Q branch of the  $2\nu_1$  band of BrNO.

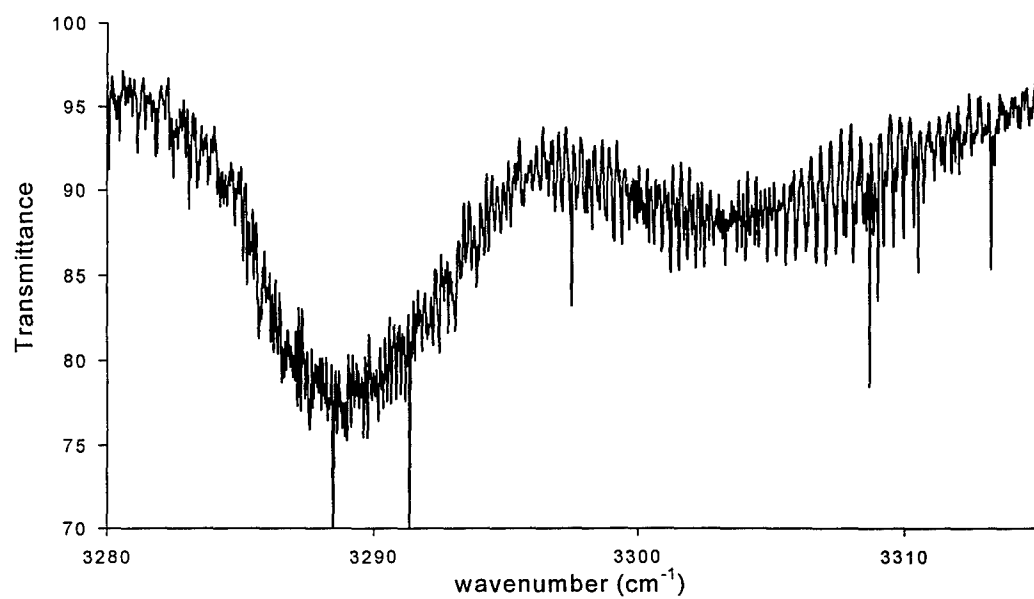


Figure 3.33 Spectrum of  $2\nu_1 - \nu_3$  band of BrNO.

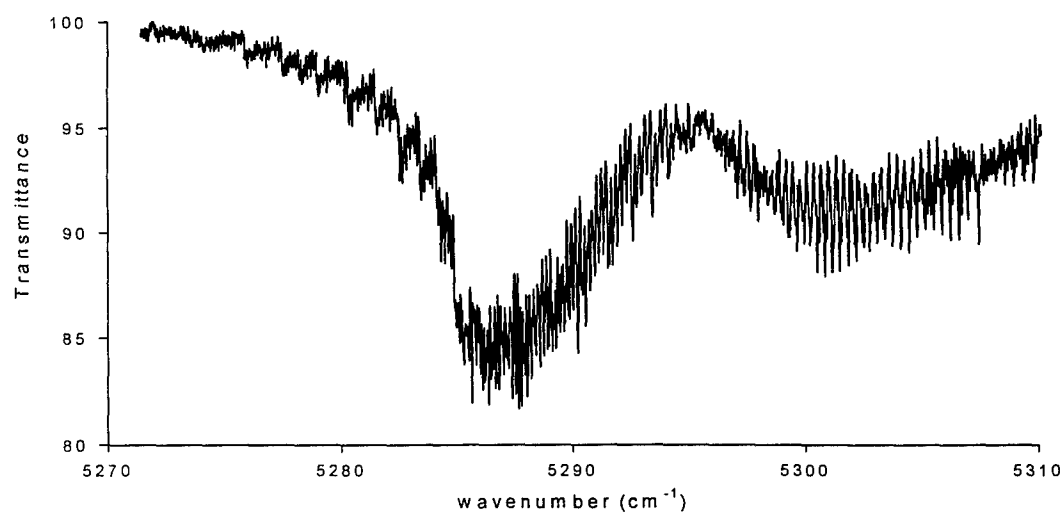


Figure 3.34 Spectrum of  $3\nu_1$  band of BrNO.

the levels may interact via a *Fermi resonance* that increases the energy difference between the levels and alters the intensities of the transitions into or out of the interacting levels. The rotational energy levels of two vibrational modes that have approximately the same energy may also be shifted by a Coriolis interaction. For nonsymmetric triatomic molecules  $\nu_1$  and  $\nu_3$  may interact with  $\nu_2$  but  $\nu_1$  and  $\nu_3$  would not be expected to interact with each other (1). First order Coriolis interactions can occur if the vibrational quantum numbers of the interacting modes differ by no more than one. If the quantum numbers differ by more than one higher order Coriolis interactions may occur.

Several of the lower vibrational levels of BrNO are nearly degenerate (Figure 3.4). The interaction of the (0,1,0) and (0,0,2) levels was noted by Laane (41). The (1,1,0) and (1,0,2) levels as well as the (2,1,0) and (2,0,2) may also be expected to interact. The interaction between the nearly coincident vibrational levels makes the analysis of the affected bands much more difficult and the analysis of these bands is incomplete.

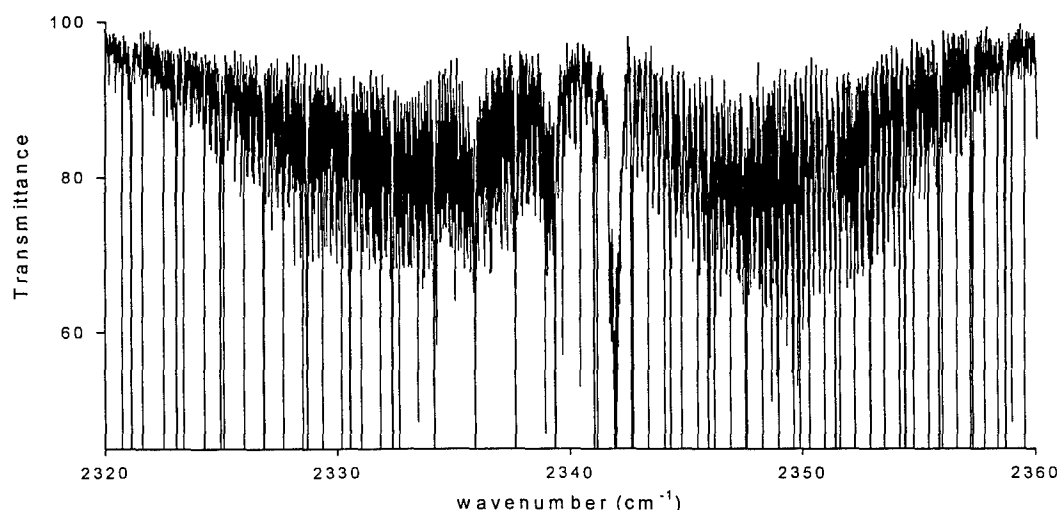


Figure 3.35 Spectrum of  $\nu_1 + \nu_2$  and  $\nu_1 + 2\nu_3$  bands of BrNO.

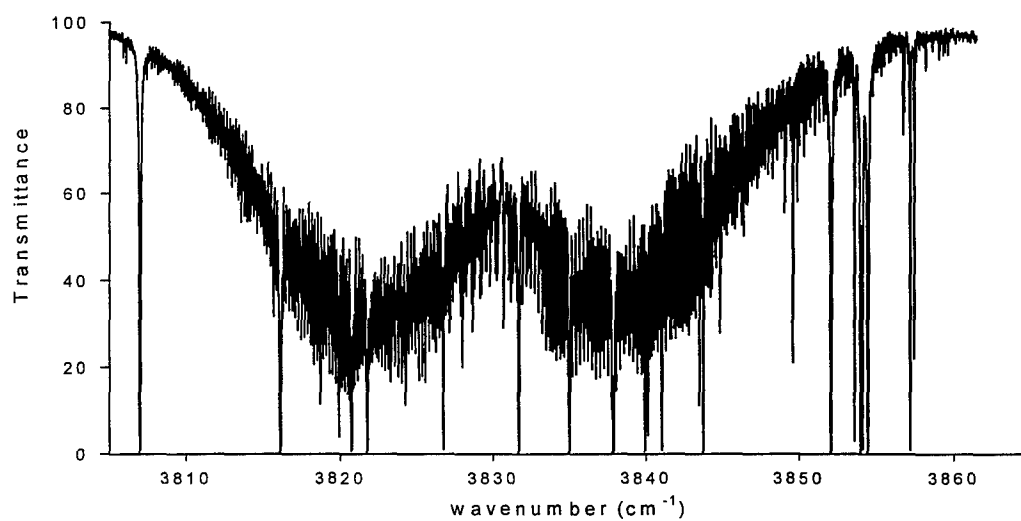


Figure 3.36 Spectrum of  $2\nu_1 + \nu_3$  band of BrNO.

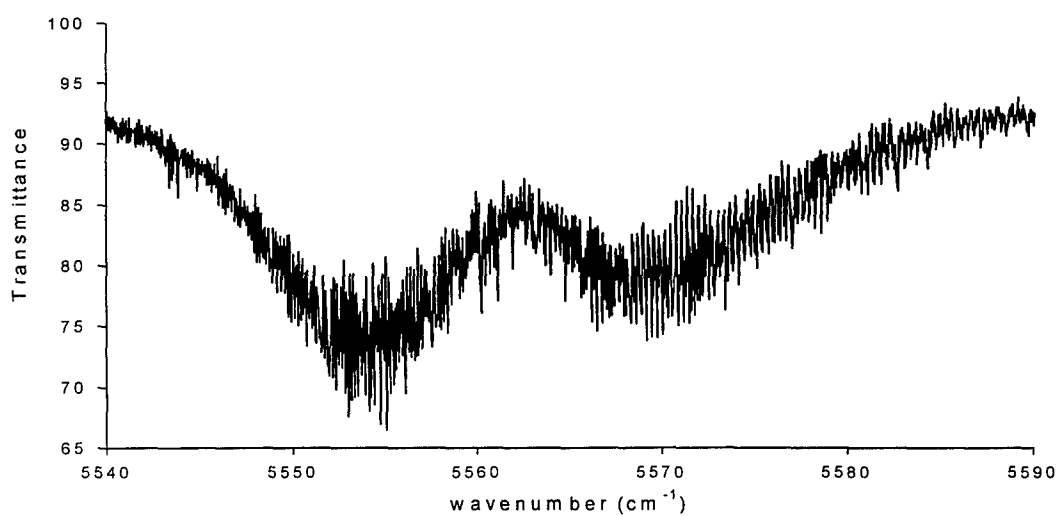


Figure 3.37 Spectrum of  $3\nu_1 + \nu_3$  band of BrNO.

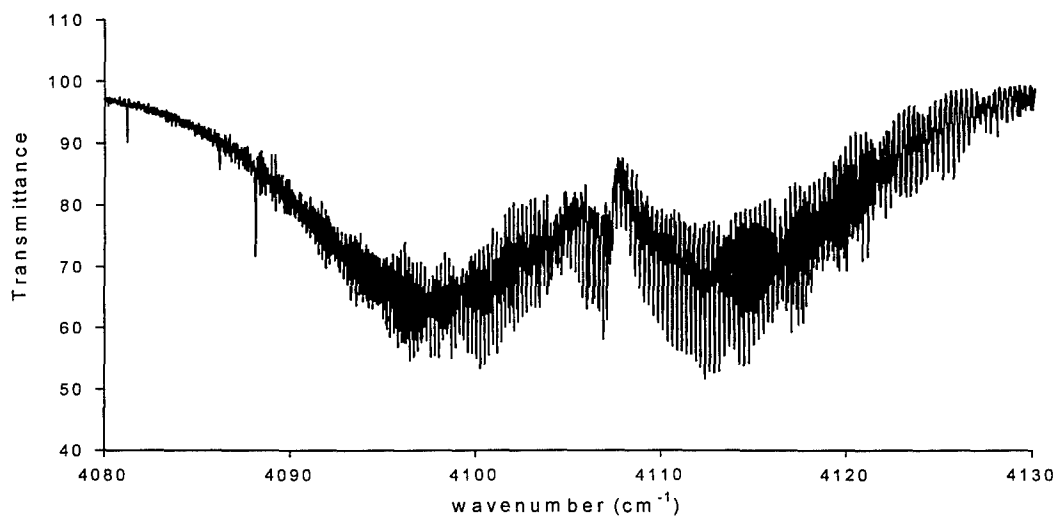


Figure 3.38 Spectrum of  $2\nu_1 + \nu_2$  and  $2\nu_1 + 2\nu_3$  bands of BrNO.

The  $\nu_1 + \nu_3$  band at  $2065\text{ cm}^{-1}$ , and the  $\nu_1 + \nu_2 - \nu_3$  hotband at  $2075\text{ cm}^{-1}$  overlap (Figure 3.39) but do not involve vibrational levels that are close enough to interact—the first is a transition from  $(0\ 0\ 0)$  to  $(1\ 0\ 1)$  while the second is from  $(0\ 0\ 1)$  to  $(1\ 1\ 0)$ .

**3.6.4 Line positions.** The observed and predicted positions of the assigned lines for each band may be found in Appendix B.

**3.6.5 Fits.** The parameter fits for the bands are listed in the following tables. The rotational and distortion constants are in MHz and the inertia defects in  $\text{amu}\ \text{\AA}^2$ . The asymmetry parameter  $\kappa$  is dimensionless. The standard errors in units of the last quoted digits are in parentheses.

The difference between the observed and predicted line positions for the  $2\nu_1$  band and the  $3\nu_1$  band are shown in Figures 3.40 and 3.41. The spectroscopic constants for the  $(0\ 0\ 1)$  level were obtained from the analysis of the  $2\nu_1 - \nu_3$  hotband, using the constants determined for the  $(2\ 0\ 0)$  level from the analysis of the  $2\nu_1$  band. The difference between the observed and predicted line positions for the



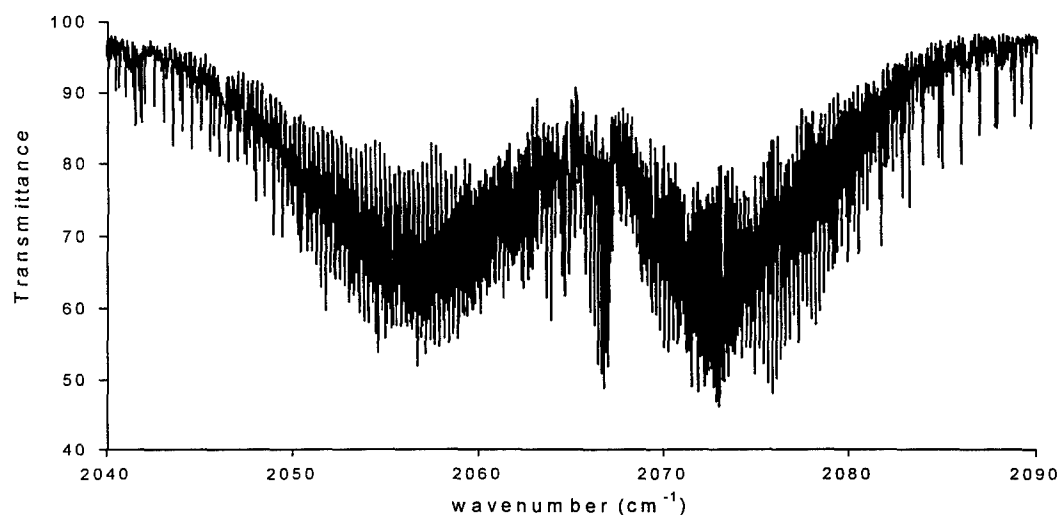


Figure 3.39 Spectrum of  $\nu_1 + \nu_3$  and  $\nu_1 + \nu_2 - \nu_3$  bands of BrNO.

Table 3.12 Observed spectroscopic constants for the (2 0 0) vibrational level of BrNO.

	$^{79}\text{BrNO}$	$\text{ON}^{81}\text{Br}$
A	83934.22 (12)	83917.20 (97)
B	3778.0780 (44)	3753.2539 (46)
C	3611.9894 (43)	3589.1876 (47)
$\kappa$	-.99586444	-.99591509
$\Delta_J (10^{-3})$	2.91790 (56)	2.8825 (52)
$\Delta_{JK} (10^{-2})$	-5.6953 (26)	-5.6717 (26)
$\Delta_K$	4.6390 (13)	4.6208 (88)
$\delta_J (10^{-4})$	1.6511 (46)	1.6290 (52)
$\delta_K (10^{-2})$	1.914 (79)	1.930 (76)
$\Delta^v$	.1298	.1327
number of lines assigned	800	719
$\chi^2$	315	286

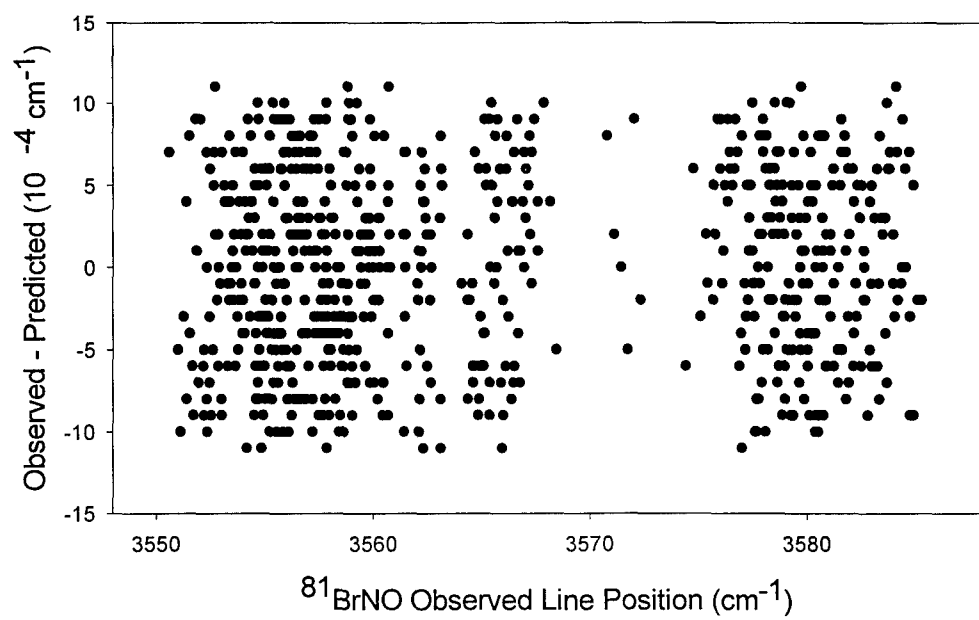
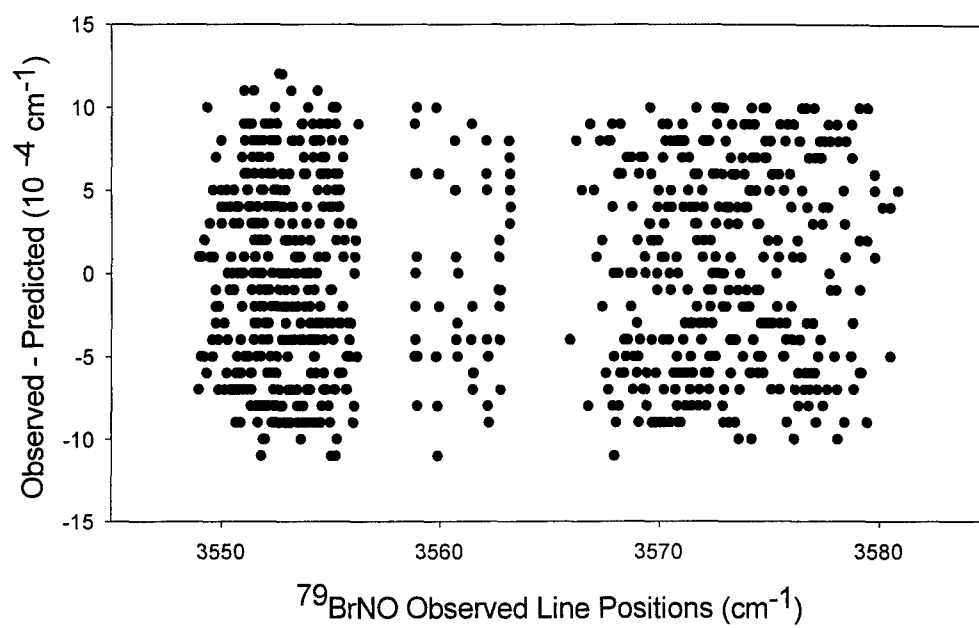


Figure 3.40 Difference between observed and predicted  $2\nu_1$  line positions for  $^{79}\text{BrNO}$  (top) and  $^{81}\text{BrNO}$  (bottom).

Table 3.13 Observed spectroscopic constants for the (3 0 0) vibrational level of BrNO.

	<sup>79</sup> BrNO	ON <sup>81</sup> Br
A	83148.20 (19)	83131.27 (12)
B	3793.5905 (72)	3768.6999 (70)
C	3625.0061 (68)	3602.1266 (73)
$\kappa$	-.995760	-.995811
$\Delta_J (10^{-3})$	2.95268 (75)	2.91447 (26)
$\Delta_{JK} (10^{-2})$	-5.7035 (49)	-5.6770 (33)
$\Delta_K$	4.5389 (17)	4.5248 (11)
$\delta_J (10^{-4})$	1.6758 (81)	1.6665 (63)
$\delta_K (10^{-2})$	2.083 (78)	1.949 (96)
$\Delta^v$	.1174	.1218
number of lines assigned	685	768
$\chi^2$	268	305

Table 3.14 Observed spectroscopic constants for the (0 0 1) vibrational level of BrNO.

	<sup>79</sup> BrNO	ON <sup>81</sup> Br
A	85981.74 (36)	85958.67 (27)
B	3729.655 (12)	3705.021 (15)
C	3568.968 (14)	3546.457 (20)
$\kappa$	-.99610	-.99615
$\Delta_J (10^{-3})$	2.8612 (10)	2.82575 (89)
$\Delta_{JK} (10^{-2})$	-5.9073 (98)	-5.871 (11)
$\Delta_K$	4.8233 (67)	4.8152 (79)
$\delta_J (10^{-4})$	1.570 (22)	1.556 (35)
$\delta_K (10^{-2})$	2.087 (93)	2.127 (69)
$\Delta^v$	.22306	.21937
number of lines assigned	278	305
$\chi^2$	127	139

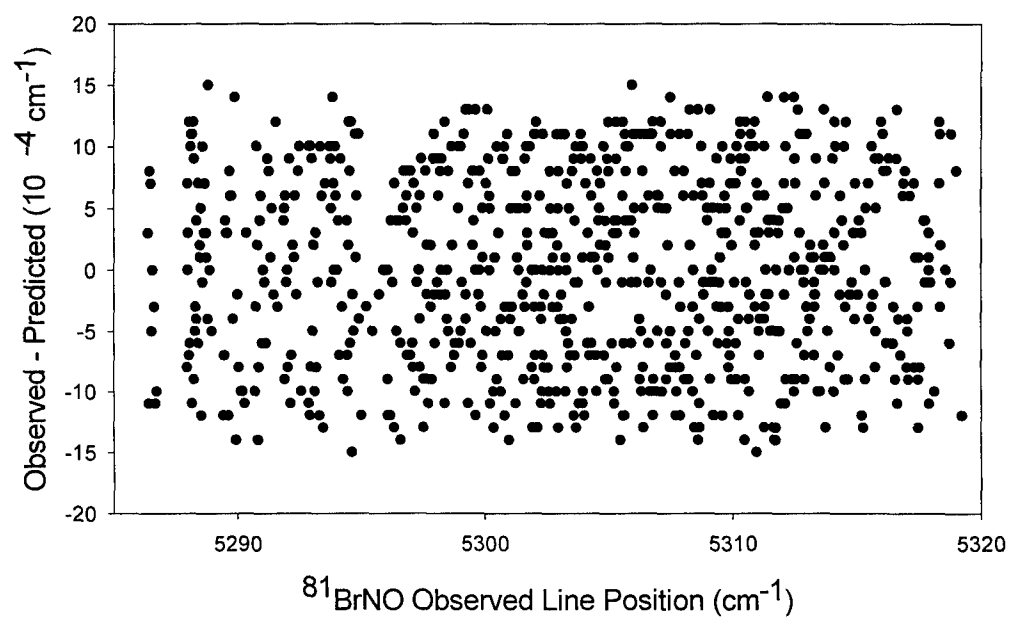
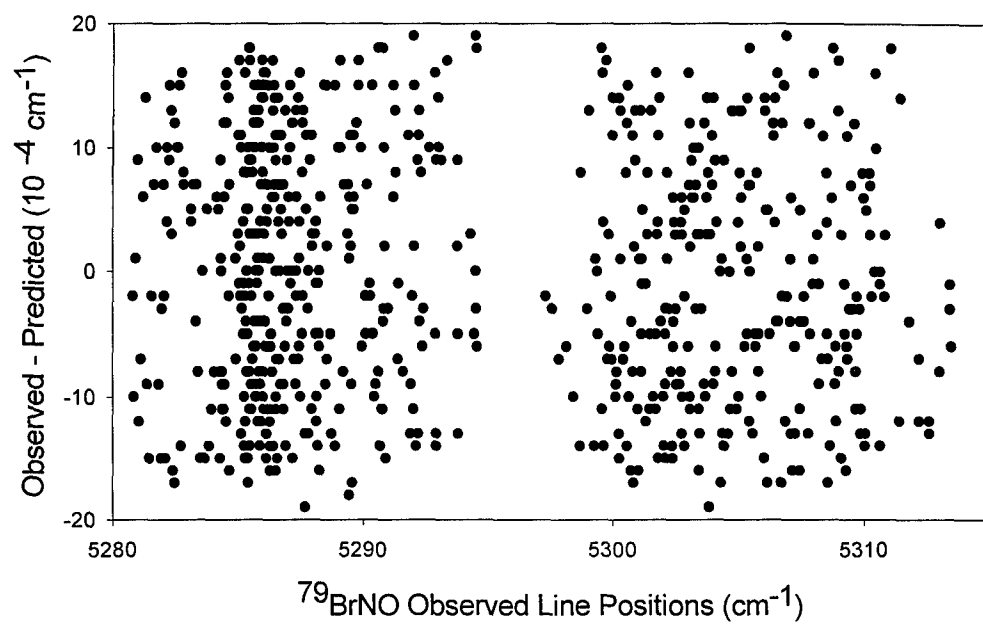


Figure 3.41 Difference between observed and predicted  $3\nu_1$  line positions for  $^{79}\text{BrNO}$  (top) and  $^{81}\text{BrNO}$  (bottom).

$2\nu_1 - \nu_3$  band are shown in Figure 3.42. The difference between the observed

Table 3.15 Observed spectroscopic constants for the (2 0 1) vibrational level of BrNO.

	$^{79}\text{BrNO}$	$\text{ON}^{81}\text{Br}$
A	83414.59 (18)	84393.15 (14)
B	3760.5712 (60)	3735.9147 (58)
C	3594.9631 (57)	3572.3406 (58)
$\kappa$	-.995851	-.99595
$\Delta_J (10^{-3})$	2.9275 (59)	2.8916 (67)
$\Delta_{JK} (10^{-2})$	-5.9109 (38)	-5.8831 (30)
$\Delta_K$	4.632 (18)	4.7272 (14)
$\delta_J (10^{-4})$	1.669 (68)	1.6367 (59)
$\delta_K (10^{-2})$	2.093 (78)	2.101 (79)
$\Delta^v$	.2036	.2061
number of lines assigned	376	388
$\chi^2$	376	207

and predicted line positions for the  $2\nu_1 + \nu_3$  band are shown in Figure 3.43.

Table 3.16 Observed spectroscopic constants for the (3 0 1) vibrational level of BrNO.

	$^{79}\text{BrNO}$	$\text{ON}^{81}\text{Br}$
A	83628.51 (86)	83607.44 (76)
B	3776.088 (13)	3751.370 (16)
C	3607.970 (20)	3585.278 (17)
$\kappa$	-.99580	-.99590
$\Delta_J (10^{-3})$	2.960 (24)	2.925 (43)
$\Delta_{JK} (10^{-2})$	-5.907 (32)	-5.891 (33)
$\Delta_K$	4.54 (10)	4.73 (14)
$\delta_J (10^{-4})$	1.696 (21)	1.675 (24)
$\delta_K (10^{-2})$	2.072 (23)	2.125 (31)
$\Delta^v$	.19315	.19632
number of lines assigned	175	186
$\chi^2$	78.3	84.6

The difference between the observed and predicted line positions for the  $3\nu_1 + \nu_3$  band are shown in Figure 3.44. No high-quality spectra of any band that would

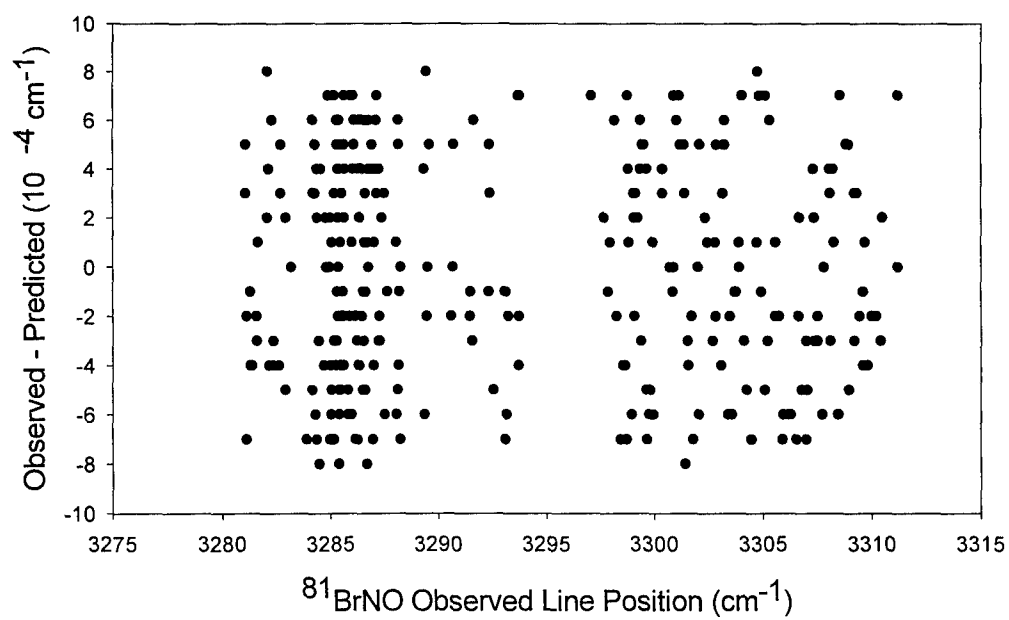
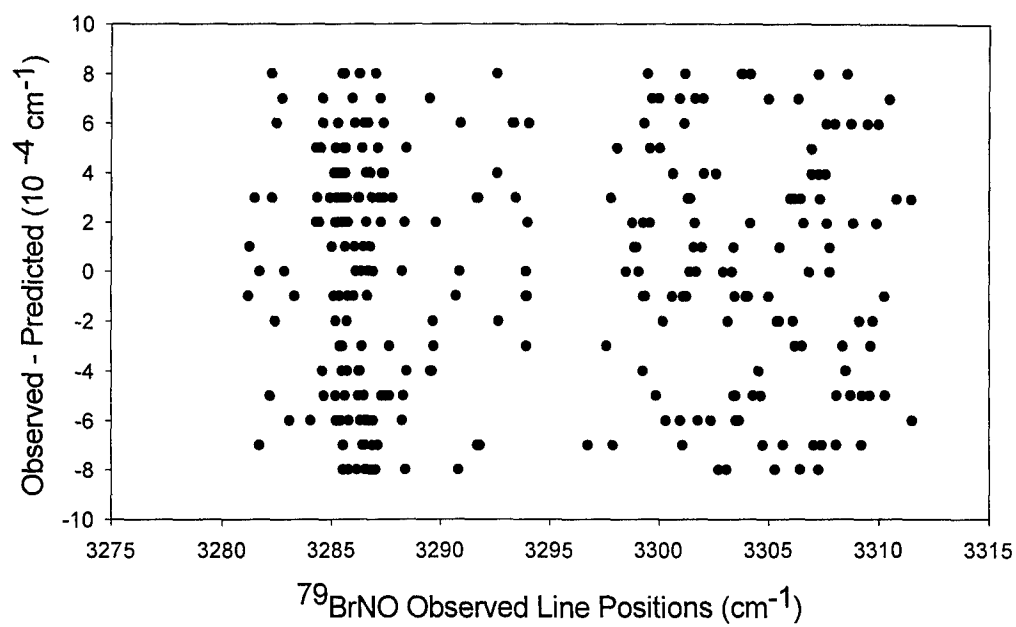


Figure 3.42 Difference between observed and predicted  $2\nu_1 - \nu_3$  line positions for  $^{79}\text{BrNO}$  (top) and  $^{81}\text{BrNO}$  (bottom).

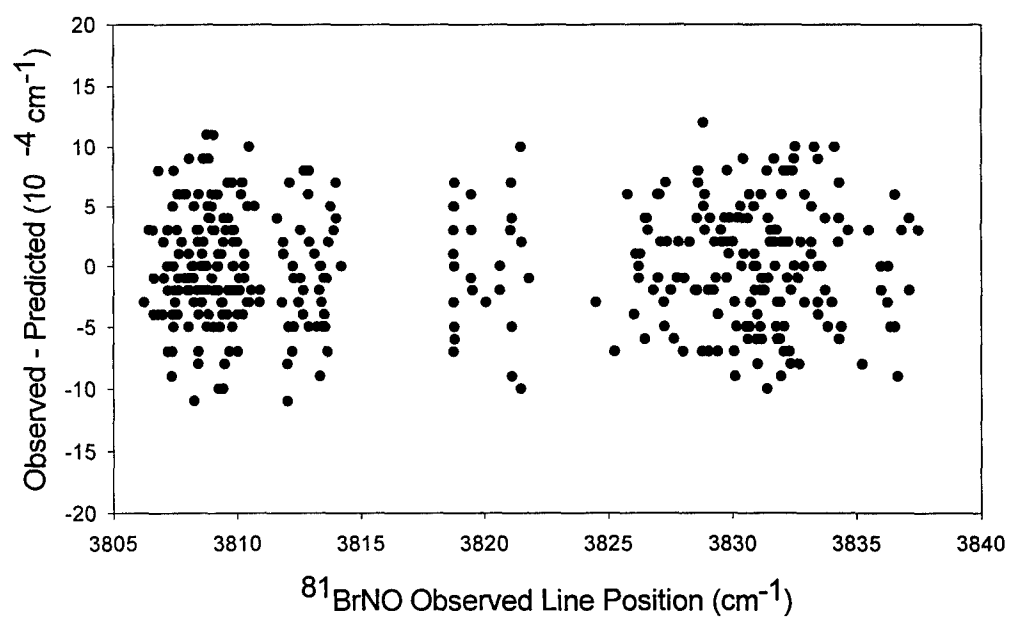
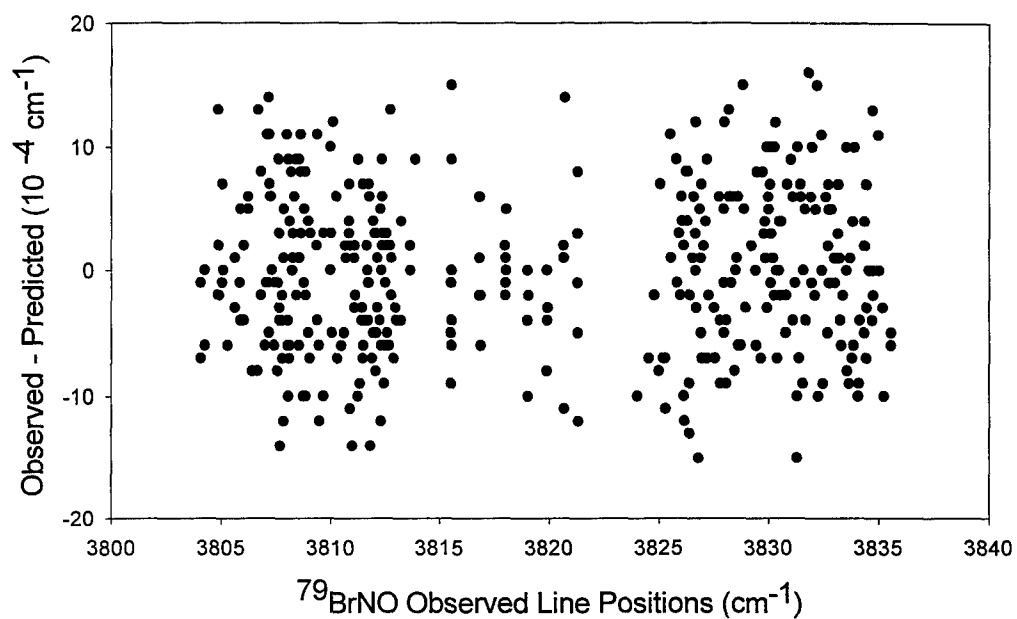


Figure 3.43 Difference between observed and predicted  $2\nu_1 + \nu_3$  line positions for  $^{79}\text{BrNO}$  (top) and  $^{81}\text{BrNO}$  (bottom).

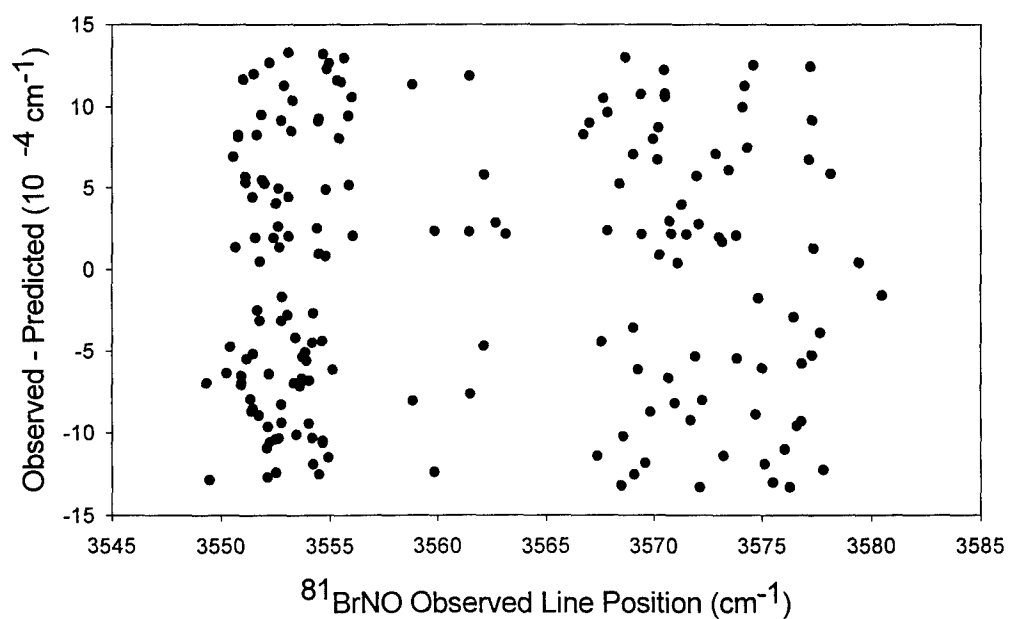
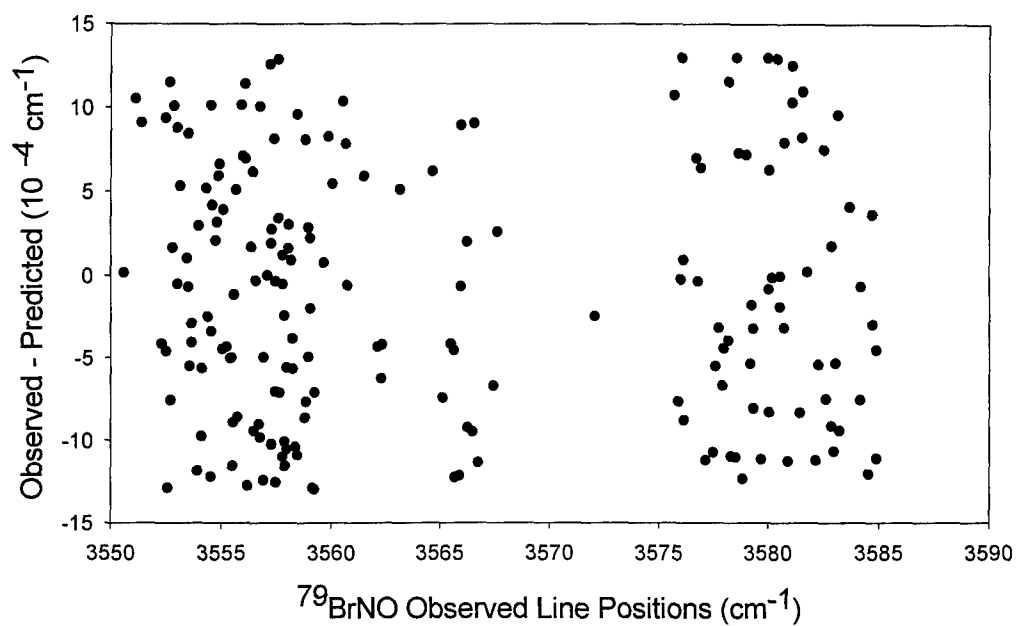


Figure 3.44 Difference between observed and predicted  $3\nu_1 + \nu_3$  line positions for  $^{79}\text{BrNO}$  (top) and  $^{81}\text{BrNO}$  (bottom).



allow the straightforward determination of the effect of changes in the  $\nu_2$  quantum number were obtained. The overlapping  $\nu_1 + \nu_3$  and  $\nu_1 + \nu_2 - \nu_3$  bands offer the best chance of obtaining some information about  $\nu_2$ , since their coincidence is accidental, but requires distinguishing the mixed lines of two bands, each of which involves two isotopes. Contaminating  $\text{H}_2\text{O}$  lines and the relative weakness of the  $\nu_1 + \nu_2 - \nu_3$  hotband increase the difficulty of the problem. The (0 0 0), (1 0 0) and (0 0 1) constants were used to estimate the (1 0 1) constants to allow the identification of the  $\nu_1 + \nu_3$  lines. Relatively few of the  $\nu_1 + \nu_2 - \nu_3$  lines could be unambiguously identified, leading to larger errors in the calculated constants. The difference between

Table 3.17 Observed spectroscopic constants for the (1 1 0) vibrational level of  $\text{BrNO}$ .

	$^{79}\text{BrNO}$	$\text{ON}^{81}\text{Br}$
A	85633.00 (13)	85619.62 (21)
B	3745.2021 (89)	3720.2134 (75)
C	3578.4556 (84)	3556.4621 (79)
$\kappa$	-.99594	-.99601
$\Delta_J (10^{-3})$	2.9007 (49)	2.9111 (56)
$\Delta_{JK} (10^{-2})$	-6.0817 (34)	-6.0412 (30)
$\Delta_K$	4.7293 (54)	4.7155 (64)
$\delta_J (10^{-4})$	1.6472 (47)	1.6127 (70)
$\delta_K (10^{-2})$	2.1842 (27)	2.1637 (47)
$\Delta^v$	.3865	.3522
number of lines assigned	109	134
$\chi^2$	89.2	154

the observed and predicted line positions for the  $\nu_1 + \nu_2 - \nu_3$  band are shown in Figure 3.45.

*3.6.6 Vibration/Rotation Interaction Terms.* The nonlinear variation of the rotational constants with increasing  $v_1$  indicates that the first order vibration/rotation interaction terms in Equation 3.27 do not completely account for the vibrational dependence of the rotational constants. More extensive data, however,

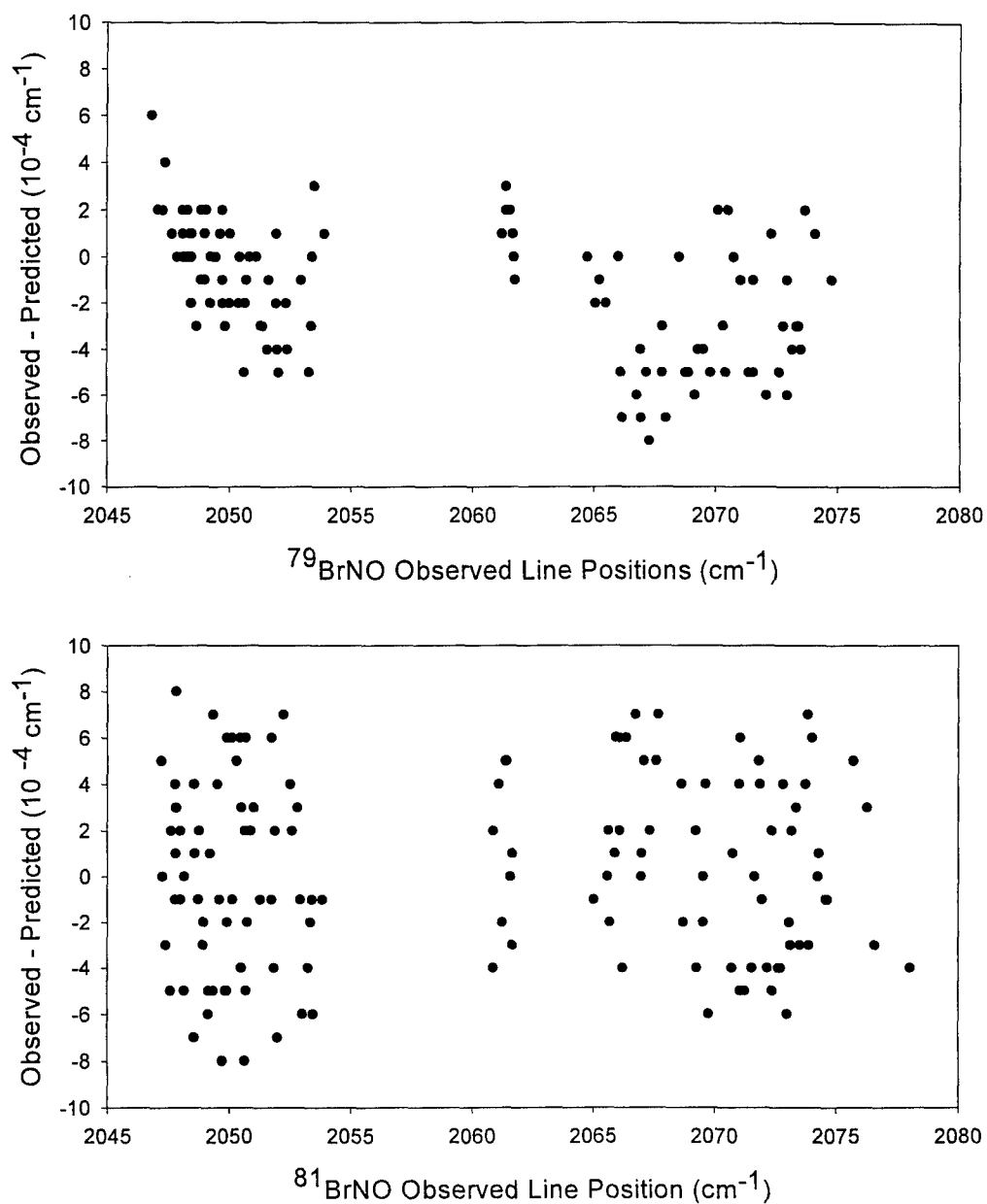


Figure 3.45 Difference between observed and predicted  $\nu_1 + \nu_2 - \nu_3$  line positions for  $^{79}\text{BrNO}$  (top) and  $^{81}\text{BrNO}$  (bottom).

is needed to quantify the second order effects. The interaction terms were calculated using only the (0 0 1) and (1 1 0) data combined with the (0 0 0) and (1 0 0) values from the literature. If  $B^{ijk}$  is one of the three rotational constants for vibrational level (i j k) the interaction terms and equilibrium values may be estimated as

$$\begin{aligned}\alpha_1^B &= B^{000} - B^{100} \\ \alpha_2^B &= B^{100} - B^{110} \\ \alpha_1^B &= B^{000} - B^{001} \\ B_e &= 2B^{000} - \frac{1}{2}B^{110} - \frac{1}{2}B^{001}\end{aligned}$$

but the values in Table 3.18 were determined using a least squares multiple regression analysis (58) that also determined the errors in the estimates.

### 3.7 Summary

In this experiment high-resolution spectra of the  $\nu_1 + \nu_3$ ,  $\nu_1 + \nu_2 - \nu_3$ ,  $2\nu_1 - \nu_3$ ,  $2\nu_1$ ,  $3\nu_1$ ,  $2\nu_1 + \nu_3$  and  $3\nu_1 + \nu_3$  ro-vibrational bands of  $^{81}\text{BrNO}$  and  $^{79}\text{BrNO}$  were analyzed and 4923 spectral lines fit using a Hamiltonian function that accounts for the effects of centrifugal distortion on the rotational energy levels of an asymmetric molecule. The rotational and quartic distortion terms, inertia defects and asymmetry parameters were determined for the (2 0 0), (3 0 0), (0 0 1), (2 0 1), (3 0 1) and (1 1 0) vibrational levels and the first-order vibration/rotation interaction terms were also determined.

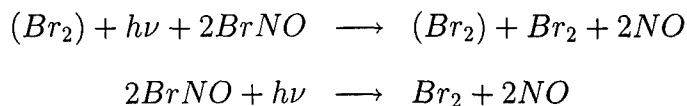
Table 3.18 Vibration/rotation interaction constants and equilibrium values of the rotation constants for  $^{79}\text{BrNO}$  and  $^{81}\text{BrNO}$ , in MHz.

	$^{79}\text{BrNO}$	$^{81}\text{BrNO}$
$\alpha_1^A$	779.7320(19)	779.854(23)
$\alpha_2^A$	-913.470(20)	-916.510(24)
$\alpha_3^A$	-481.278(20)	-475.726(24)
$\alpha_1^B$	-15.53337(44)	-15.45392(53)
$\alpha_2^B$	17.40390(44)	17.59170(54)
$\alpha_3^B$	17.41553(44)	17.32678(54)
$\alpha_1^C$	-12.99545(47)	-12.94306(59)
$\alpha_2^C$	20.53333(48)	19.79200(60)
$\alpha_3^C$	17.01985(48)	16.85194(60)
$A_e$	85192.9540(99)	85176.753(12)
$B_e$	3756.71356(22)	3732.08010(52)
$C_e$	3598.26670(24)	3575.15940(30)

#### IV. Conclusion

The kinetics of BrNO formation and destruction have been examined using time-resolved photolysis techniques. The equilibrium constant for the dark reaction  $\text{Br}_2 + 2\text{NO} \rightleftharpoons 2\text{BrNO}$  was determined as  $K_{\text{eq}} = 168 \pm 23 \text{ atm}^{-1}$  and the rate constant for the forward reaction as  $k_f = 1.40 \pm .18 \times 10^{-38} \text{ cm}^6/\text{molecule}^2\text{-s}$  at 293K. A novel technique for the fitting of the observed time profiles to the three-body kinetics was developed which utilizes the complete temporal profile to establish the rate coefficients. The agreement between the data and the model demonstrated by the new fitting technique provides further evidence that the reaction of  $\text{Br}_2$  and NO is adequately described by third-order kinetics. The values of the rate constants are consistent with those determined previously.

When an equilibrium mixture of  $\text{Br}_2$ , NO and BrNO is disturbed by photolysis, BrNO is rapidly removed by reaction with atomic bromine. For continuous photolysis, a new photostationary condition is achieved which shifts the equilibrium toward  $\text{Br}_2$  and NO. If the new BrNO concentration is not zero the steady-state Br concentration will be very small; the bromine atoms liberated by photodissociation of  $\text{Br}_2$  and BrNO are immediately converted into  $\text{Br}_2$  and NO by a kinetic mechanism equivalent to:



The photolysis of  $\text{Br}_2$  in conjunction with the reaction of Br atoms with BrNO gives a net gain of one bromine molecule and two NO molecules for each bromine molecule dissociated. The simultaneous photolysis of BrNO results in the destruction of BrNO with a quantum yield of 2. This kinetic mechanism and rates for the photolysis of mixtures of  $\text{Br}_2$ , NO and BrNO has been validated for total pressures of 28-111 torr

and nitric oxide to molecular bromine concentration ratios of 2.18-26.75, with an average  $\text{Br}_2$  photolysis rate of 0.050 molecules/s.

These results must now be applied to the characterization of the performance of the  $\text{Br}(^2\text{P}_{1/2})\text{-NO}(v=2 \rightarrow v=1)$  transfer laser pumped by photolysis of iodine molecules, and their implications with respect to the destruction of stratospheric ozone must be explored.

The rotation structure of the  $\nu_1 + \nu_2 - \nu_3$ ,  $2\nu_1 - \nu_3$ ,  $2\nu_1$ ,  $3\nu_1$ ,  $2\nu_1 + \nu_3$  and  $3\nu_1 + \nu_3$  overtone and combination bands of  $\text{BrNO}$  were examined at high resolution ( $.005 - .01 \text{ cm}^{-1}$ ) using Fourier Transform Spectroscopy. Over 4900 spectral lines were recorded for the two isotopes  $^{79}\text{BrNO}$  and  $^{81}\text{BrNO}$ . The rotational and quartic distortion terms, inertia defects and asymmetry parameters were determined for the (200), (300), (001), (200), (301) and (110) vibrational levels. The first-order vibration-rotation interaction terms were also determined.

All of these quantities are intimately tied to fundamental molecular properties. The next phase of this research is a detailed analysis of those properties.

## Bibliography

1. Allen, Harry C. and Paul B. Cross. *Molecular Vib-Rotors*. New York: John Wiley and Sons, 1963.
2. Asimov, Isaac. *Asimov's Biographical Encyclopedia of Science and Technology* (2<sup>nd</sup> Edition). Garden City, New York: Doubleday and Company, 1982.
3. Barrow, Gordon M. *Introduction to Molecular Spectroscopy*. New York: McGraw-Hill, 1962.
4. Baulch, D. L., editor. *Journal of Physical and Chemical Reference Data*. New York: American Institute of Physics, 1981.
5. Bell, Robert J. *Introductory Fourier Transform Spectroscopy*. New York: Academic Press, 1972.
6. Boggs, James E., et al. "Systematic ab Initio Gradient Calculation of Molecular Geometries, Force Constants, and Dipole Moment Derivatives," *Journal of the American Chemical Society*, 101(10):2550-2560 (1979).
7. Bomem, Inc. *Spectrometer System Manual*. Bomem, Inc, Quebec, 1990.
8. Bransden, B. H. and C. J. Joachain. *Physics of Atoms and Molecules*. Essex: Longman Scientific and Technical, 1983.
9. Brigham, E. O. *The Fast Fourier Transform*. Englewood Cliffs, N.J.: Prentice-Hall, 1974.
10. Burns, W. G. and H. J. Bernstein. "The Vibrational Spectra and Structure of Inorganic Molecules. III. The Infrared Spectra of Nitrosyl Chloride and Nitrosyl Bromide from 2.0 to 2.5  $\mu\text{m}$ ," *Journal of Chemical Physics*, 18:1669-1673 (1950).
11. Cole, A. R. H. *Tables of Wavenumbers for the Calibration of Infrared Spectra*. Oxford: Pergamon Press, 1977.
12. Degli Eposti, C., et al. "High-resolution Fourier Transform Spectroscopy of the  $\nu_1$  Fundamental Band of Nitrosyl Bromide," *Chemical Physics Letters*, 214:531-535 (1993).
13. Degli Eposti, C., et al. "Centrifugal Distortion and Hyperfine Structure Analysis of the Millimeter-Wave Spectrum of Nitrosyl Bromide," *Journal of Molecular Spectroscopy*, 163:313-325 (1994).
14. DeGraff, B. A. and K. J. Lang. "Gas-Phase Recombination of Bromine Atoms," *Journal of Physical Chemistry*, 74:4181-4186 (1970).
15. del Barrio, J. I., et al. "New Chemical Laser from the Photodissociation of  $\text{BrNO}$ ," *Optics Communications*, 55:280-282 (1985).

16. del Barrio, J. I., et al. "Temporal Behavior of NO Laser Emission from the Photodissociation of ClNO and BrNO," *Journal of Applied Physics*, 59:4184-4186 (1986).
17. del Barrio, J. I. and F. M. G. Tablas. "Relative Intensities of the NO Vibro-Rotational Laser Transitions from the Photodissociation of BrNO," *Optics Communications*, 58:245-248 (1986).
18. Donald F. Eagle, T. L. Weatherly and Quitman Williams. "Stark Effect in the Microwave Spectrum of Nitrosyl Bromide,"
19. Dowling, J. M. "Centrifugal Distortion in Planar Molecules," *Journal of Molecular Spectroscopy*, 6:550-553 (1961).
20. Fleissner, Gerhard, et al. "Improved Curve Resolution of Highly Overlapping Bands by Comparison of Fourth-Derivative Curves," *Applied Spectroscopy*, 50(10):1235-1245 (1996).
21. Griffiths, Peter R. and James A. de Haseth. *Fourier Transform Infrared Spectrometry*. New York: Wiley Interscience, 1986.
22. Grimley, A. J. and P. L. Houston. "Photochemistry of Nitrosyl Halides: the  $X + NOX \Rightarrow X_2 + NO$  (v) Reaction (  $X = Cl, Br$ )," *Journal of Chemical Physics*, 72:1471-1475 (1980).
23. Guelachvili, G. and K. Narahari Rao, editors. *Handbook of Infrared Standards*. New York: Academic Press, 1986.
24. Hargittai, István and Magdolna Hargittai. *Symmetry through the Eyes of a Chemist*. New York: Plenum Press, 1995.
25. Harris, Daniel C. and Michael D. Bertolucci. *Symmetry and Spectroscopy—An Introduction to Vibrational and Electronic Spectroscopy*. New York: Oxford University Press, 1978.
26. Haugen, H. K., et al. "Accurate Quantum Yields by Laser Gain versus Absorption Spectroscopy: Investigation of Br/Br\* Channels in Photofragmentation of Br<sub>2</sub> and IBr," *Journal of Chemical Physics*, 83:3402-3412 (1985).
27. Hawks, M. R., et al. "Infrared fluorescence study of electronic-to-vibrational energy transfer in the Br(<sup>2</sup>P<sub>1/2</sub>) - NO System," *Chemical Physics*, 195:395-401 (1995).
28. Herzberg, G. *Infrared and Raman Spectra II. Infrared and Raman Spectra of Polyatomic Molecules*. New York: Van Nostrand Reinhold Company, 1945.
29. Herzberg, G. *The Spectra and Structure of Simple Free Radicals*. Ithaca, New York: Cornell University Press, 1971.
30. Hippler, H., et al. "Flash Photolysis Study of the NO-Catalyzed Recombination of Bromine Atoms," *International Journal of Chemical Kinetics*, 10:155-169 (1978).



31. Hisatsune, I. C. and Leo Zafonte. "A Kinetic study of Some Third-Order Reactions of Nitric Oxide," *Journal of Physical Chemistry*, 73:2980-2989 (1969).
32. Houel, N. and H. van den Bergh. "BrNO-Thermodynamic Properties, the Ultra-violet/Vis Spectrum, and the Kinetics of Its Formation," *International Journal of Chemical Kinetics*, IX:867-874 (1977).
33. Ip, J. K. K. and George Burns. "Recombination of Br Atoms by Flash Photolysis Over a Wide Temperature Range. II. Br<sub>2</sub> in He, Ar, Kr, N<sub>2</sub> and O<sub>2</sub>," *Journal of Chemical Physics*, 51:3414-3424 (1969).
34. Jim Smith, Melles Griot engineer. Personal communication, May 1997.
35. Johnson, Ray O. *Excited Atomic Bromine Energy Transfer and Quenching Mechanisms*. PhD dissertation, Air Force Institute of Technology, Wright-Patterson AFB, OH, 1993.
36. King, G. W., et al. "The Asymmetric Rotor I. Calculation and Symmetry Classification of Energy Levels," *Journal of Chemical Physics*, 11:27-42 (1943).
37. Kivelson, D. and Jr. E. B. Wilson. "Approximate Treatment of the Effect of Centrifugal Distortion on the Rotational Energy levels of Asymmetric Top Molecules," *Journal of Chemical Physics*, 20:1575-1579 (1952).
38. Klotz, Irving M. and Robert M. Rosenberg. *Chemical Thermodynamics*. Menlo Park, California: Benjamin/Cummings Publishing Company, 1986.
39. Krauss, W. Z. *Phys. Chem.*, A175:295 (1936). reported in Houel (32).
40. Kroto, H. W. *Molecular Rotation Spectra*. New York: Wiley, 1975. Available as a Dover paperback.
41. Laane, J., et al. "Vibrational Spectra and Force Constants for Isotopic Species of Nitrosyl Bromide," *Journal of Molecular Spectroscopy*, 30:485-497 (1969).
42. Laidler, Keith J. *Chemical Kinetics*. New York: McGraw-Hill, 1965.
43. Maddams, W. F. *Applied Spectroscopy*, 34 (1980).
44. Maki, Jr., Arthur G. "Vibrational Spectroscopy." *Annual Reviews of Physical Chemistry*, 20 273-289.
45. Marshall, Alan G., editor. *Fourier, Hadamard, and Hilbert Transforms in Chemistry*, 387-420. New York: Plenum Press, 1982.
46. Mills, I. M. "Vibration-Rotation Structure in Asymmetric and Symmetric-Top Molecules." *Molecular Spectroscopy Modern Research* New York: Academic Press, 1972.
47. MKS Instruments, Inc., Andover, Massachusetts. *Type 690 and 698 High Accuracy Pressure Transducers*, 1992.
48. M.W. Chase, Jr., et al. *JANAF Thermochemical Tables*. American Chemical Society, 1985.

49. Okabe, Hideo. *Photochemistry of Small Molecules*. New York: Wiley Interscience, 1978.
50. Oriel Corporation, Stratford, CT. *Oriel Catalogue* (Volumn ii Edition), 1994.
51. Parkinson, Claire L. *Breakthroughs-A Chronology of Great Achievements in Science and Mathematics*. Boston: G. K. Hall and Company, 1985.
52. Perram, G. *Applied Physics B* To be published Summer 1997.
53. Perram, G. Personal communication, April 1997.
54. Perram, G.P., et al. "Radial diffusion between coaxial cylinders and surface deactivation of  $O_2(b^1\Sigma_g^+)$ ," *Chemical Physics*, 162:427-432 (1992).
55. Petersen, A. B., et al. " $H_2O$ , NO and  $N_2O$  Infrared Lasers Pumped Directly and Indirectly by Electronic- vibrational Energy Transfer," *Journal of Applied Physics*, 48:230-233 (1977).
56. Peterson, A. B., et al. "Infrared Molecular Lasers Pumped by Electronic-Vibrational Energy Transfer from  $Br(4^2P_{1/2})$ :  $CO_2$ ,  $N_2O$ , HCN, and  $C_2H_2$ ," *Applied Physics Letters*, 27:305-306 (1979).
57. Pickett, Herbert M. "The Fitting and Prediction of Vibration-Rotation Spectra with Spin Interactions," *Journal of Molecular Spectroscopy*, 148:371-378 (1991).
58. Press, W. H., et al. *Numerical Recipes in Fortran 77: The Art of Scientific Computing*. Cambridge: Cambridge University Press, 1992.
59. Sedlacek, Arthur J. and Charles A. Wight. "Infrared Fluorescence Study of E-V Energy Transfer from  $Br^*(4P^{1/2})$  to Nitrosyl Bromide," *Journal of Chemical Physics*, 86:2787-2792 (1987).
60. Seery, D. J. and D. Britton. "The Continuous Absorption Spectrum of Chlorine, Bromine, Bromine Chloride, Iodine Chloride, and Iodine Bromide," *Journal of Physical Chemistry*, 68:2263-2266 (1964).
61. Steinfeld, Jeffrey I., et al. *Chemical Kinetics and Dynamics*. Englewood Cliffs, NJ: Prentice-Hall, 1989.
62. Theophanides, T., editor. *Introduction to Dispersive and Interferometric Infrared Spectroscopy*, 25-42. Dordrecht, Holland: D. Reidel Publishing Company, 1984.
63. Ulrich Magg, Josef Lindenmayer and Harold Jones. "Diode Laser Spectroscopy of the  $\nu_1$  and  $\nu_3$  Bands of Thiazyl Fluoride (FSN)," *Journal of Molecular Spectroscopy*, 126:270-281 (1987).
64. Watson, J. K. G. "Determination of Centrifugal Distortion Coefficients of Asymmetric Top Molecules," *Journal of Chemical Physics*, 46:1935-1949 (1967).

65. Watson, J. K. G. "Determination of Centrifugal Distortion Coefficients of Asymmetric Top Molecules. II. Dreizler, Dendl and Rudolph's Results," *Journal of Chemical Physics*, 48:181-185 (1968).
66. Watson, J. K. G. "Determination of Centrifugal Distortion Coefficients of Asymmetric Top Molecules. III. Sextic Coefficients," *Journal of Chemical Physics*, 48:4517-4524 (1968).
67. Watson, J. K. G. "Aspects of Quartic and Sextic Centrifugal Effects on Rotational Energy Levels." *Vibrational Spectra and Structure* 6, edited by James R. Durig, 1-89, Amsterdam: Elsevier, 1977.
68. Watson, J. K. G. "A Planarity Relation for Sextic Centrifugal Distortion Constants," *Journal of Molecular Spectroscopy*, 65:123-133 (1977).
69. Weast, Robert C., editor. *CRC Handbook of Chemistry and Physics* (56th Edition). Cleaveland, Ohio: CRC Press, 1975.
70. Weist, Todd. *High Resolution Fourier Transform Spectroscopy of the First Overtone of the NO Stretch in Nitrosyl Bromide*. MS thesis, Air Force Institute of Technology, Wright-Patterson AFB, OH, 1994.
71. White, J. U. *J. Opt. Soc. Amer.*, 32 (1942).
72. Wight, Charles A. "Infrared Fluorescence Studies of Near-Resonant Electronic-to-Vibrational Energy Transfer Collisions:  $\text{Br}(4P^{1/2}) + \text{NO}$ ," *Journal of Physical Chemistry*, 90:2683-2687 (1986).
73. Wilson, E. B., et al. *Molecular Vibrations*. New York: McGraw-Hill, 1951.
74. Wolfe, William L. and George J Zissis, editors. *The Infrared Handbook* (Revised Edition). Washington, DC: Office of Naval Research, Department of the Navy, 1985.

## Appendix A. Program Used to Diagonalize the Hamiltonian Matrix

### A.1 Description of Program

A Fortran computer program was used to fit the Hamiltonian constants to the observed line positions. The computer program diagonalizes the Hamiltonian matrix discussed in Section 3.2.3 and then minimizes the nondimensional quantity

$$\chi^2 = \sum_{i=1}^N \left( \frac{y_i - y(x_i; a_1 \dots a_M)}{\sigma_i} \right)^2 \quad (\text{A.1})$$

where  $y_i$  is the measured position of spectral line  $i$ ,  $N$  is the number of observed lines,  $y(x_i; a_1 \dots a_M)$  is the position of line  $i$  predicted using the energy levels resulting from the diagonalization of the Hamiltonian matrix and  $\sigma_i$  is the error in the measurement of the line position. The predicted line positions are a function of  $x_i$  (the  $J$ ,  $K_a$  and  $K_c$  values that identify the upper and lower energy levels) and  $a_1 \dots a_M$ , the parameters in the Hamiltonian. The program performs the nonlinear fit using a singular value decomposition (SVD) routine incorporating the *Levenberg-Marquardt method* (58). The program lists the difference between the observed and predicted line positions and provides other data required to judge the goodness of the fit, including the final  $\chi^2$  value and the correlation matrix. The fitting routine can be bypassed and the program used to predict line positions but it provides no information on the intensity of the absorption lines.

### A.2 Input File Example

```
.001,1,.001,0.0    !Fitting parameters marq, debug, delchi, delgrad
31,1,1             !# of total parameters, 0 = fit 1 = predict, max # iterations
'A',1             !Reduction ('A' or 'S'), representation (Ir = 1)
85979.9,1          !A'' (MHz) (for all parameters 1 = fit, 0 = hold constant)
3729.5279,1        !B''
3568.9898,1        !C''
85633.9,0          !A'
```

```

3745.1079,0      !B'
3578.5798,0      !C'
62206935,1       !band origin in MHz
0.0028612,1      !DJ''
0.0029004,0      !DJ'
-0.0590625,1     !DJK''
-0.0607595,0     !DJK'
4.8264,1         !DK''
4.73174,0        !DK'
0.000159,1       !d1''
0.0001644,0      !d1'
0.02087,1        !d2''
0.020093,0       !d2'
0.0000000004064,0 !HJ''
0.0000000004064,0 !HJ'
0.00000012,1     !HJK''
0.00000014941,0  !HJK'
-0.0000332,1     !HKJ''
-0.000029731,0   !HKJ'
0.00103800000,0  !HK''
0.00103800000,0  !HK'
0.0000000002173,0 !h1''
0.0000000002173,0 !h1'
0.00000001672,0  !h2''
0.00000001672,0  !h2'
0.00002148,0     !h3''
0.00002148,0     !h3'
1,10,4,6,0,10,4,7,3563.22069,1,1
1,9,4,5,0,9,4,6,3563.20167,1,1
1,8,4,4,0,8,4,5,3563.18454,1,1
1,7,4,3,0,7,4,4,3563.16932,1,1
1,6,4,2,0,6,4,3,3563.156,1,1
8,8,8,8,8,8,8,8,8888.8888,1,1 !ends list of transitions

```

!1=upper vib. level,J,Ka,Kc; 0=lower vib level,J,Ka,Kc,Obs,weight,1=cm-1

### A.3 Output File Example

```

number of transitions = 719
number of fitted parameters = 9
****

```

```

CHI**2= 0.2860612E+03
PREV.GRAD= 0.2298183E+10
MARQ= 0.10E-03
# 1 X= 0.83923190E+05 PREV.GRAD= 0.2210636E+03
# 2 X= 0.37532537E+04 PREV.GRAD= 0.3022003E+06
# 3 X= 0.35891877E+04 PREV.GRAD= -0.3575233E+05
# 4 X= 0.10684439E+09 PREV.GRAD= 0.7332747E+02
# 5 X= 0.28825227E-02 PREV.GRAD= -0.1827340E+08
# 6 X= -0.56718399E-01 PREV.GRAD= -0.6059824E+07
# 7 X= 0.46207864E+01 PREV.GRAD= 0.6390344E+06
# 8 X= 0.16288494E-03 PREV.GRAD= -0.2298102E+10
# 9 X= 0.19292177E-01 PREV.GRAD= -0.8350998E+06

```

TRANSITION									FREQ. EXPERI	FREQ. CALC.	DIFFERENCE
1	1	45	0	45	0	46	0	46	3554.76210	3554.76153	0.0006
2	1	14	0	14	0	15	0	15	3560.50370	3560.50293	0.0008
3	1	44	0	44	0	45	0	45	3554.91870	3554.91926	-0.0006
4	1	15	0	15	0	16	0	16	3560.28910	3560.28911	0.0000
5	1	43	0	43	0	44	0	44	3555.07840	3555.07876	-0.0004
6	1	42	0	42	0	43	0	43	3555.24020	3555.24002	0.0002
7	1	16	0	16	0	17	0	17	3560.07710	3560.07725	-0.0002
8	1	41	0	41	0	42	0	42	3555.40270	3555.40306	-0.0004
9	1	17	0	17	0	18	0	18	3559.86670	3559.86736	-0.0007
10	1	40	0	40	0	41	0	41	3555.56750	3555.56787	-0.0004

\*\*\*\*\*

REDUCTION SCHEME = A

```

1 A(0) = 85482.8500 ( 0. ) !held constant
2 B(0) = 3722.35040 ( 0. )
3 C(0) = 3563.30690 ( 0. )
4 A(1) = 83923.1955 ( 0.9656E-01) !fitted
5 B(1) = 3753.25391 ( 0.4594E-02)
6 C(1) = 3589.18762 ( 0.4720E-02)
7 vo = 106844387. ( 1.757 )
8 DJ(0) = 0.281625000E-02( 0. )
9 DJ(1) = 0.288254476E-02( 0.5194E-06)

```

```

10 DJK(0)=      -0.566090500E-01(      0.      )
11 DJK(1)=      -0.567172423E-01(  0.2564E-04)
12 DK(0) =      4.81060000      (      0.      )
13 DK(1) =      4.62083065      (  0.8784E-03)
14 d1(0) =      0.154938000E-03(      0.      )
15 d1(1) =      0.162900569E-03(  0.5214E-06)
16 d2(0) =      0.195700000E-01(      0.      )
17 d2(1) =      0.193036013E-01(  0.7560E-03)
18 HJ(0) =      0.401100000E-09(      0.      )
19 HJ(1) =      0.401100000E-09(      0.      )
20 HJK(0)=      0.146900000E-06(      0.      )
21 HJK(1)=      0.146900000E-06(      0.      )
22 HKJ(0)=     -0.294250000E-04(      0.      )
23 HKJ(1)=     -0.294251000E-04(      0.      )
24 HK(0) =      0.103400000E-02(      0.      )
25 HK(1) =      0.103400000E-02(      0.      )
26 h1(0) =      0.212200000E-09(      0.      )
27 h1(1) =      0.212200000E-09(      0.      )
28 h2(0) =      0.163900000E-07(      0.      )
29 h2(1) =      0.163900000E-07(      0.      )
30 h3(0) =      0.212800000E-04(      0.      )
31 h3(1) =      0.212800000E-04(      0.      )

```

```

1.0                      !correlation matrix
0.0  1.0
0.1 -0.7  1.0
-0.6 -0.2 -0.3  1.0
0.0  0.5  0.0 -0.4  1.0
0.7  0.0  0.2 -0.5  0.0  1.0
0.9  0.0  0.1 -0.4  0.0  0.5  1.0
-0.1  0.8 -0.8  0.1  0.0 -0.1 -0.1  1.0
0.0  0.4 -0.4  0.0  0.7 -0.1  0.0  0.0  1.0

```

```

rms=  5.6416584195796D-04 sigma= 16.913266448366 chsq= 286.05858195343
grad= 292911.67555783 iter=  5

```

#### A.4 Program Listing

```

c
*****
c This program performs a non-linear least squares fit for
c an asymmetric top type molecule.

```

```

c Matt Elrod May 21, 1990
c Revised July 13, 1990 for speed
*****
c
c VARIABLE DECLARATION
c
      integer paf(40),tnum,nl(3000),nu(3000),ju(3000),jl(3000)
      INTEGER NUU,NLU,JUU,JLU,KOUU,KOLU,KPUU,KPLU
      integer i1,i2,panum,maxfn,err,debug,pred,rap
      integer first,iter,xnum,kpl(3000),kpu(3000),temp1,cm(3000)
      integer kol(3000),kou(3000),ie(3000,5),iso(3000),nfit(6),enum
      double precision tra(3000),res(3000),marq,chsq,delchi,delgrad
      double precision grad,utr(3000),upa(40),pa(40),rms,TRAU,CALIB
      double precision alphin(40,40),sigma,b(3000),e(3000,3),de(3000)
      character*6 pname(31)
      character*1 rid
      common /obs/tra,nl,nu,ju,jl,utr,de,ie,enum,first,b,paf,iso,
+ kpu,kpl,kou,kol,temp1
      data pname/'A(0)', 'B(0)', 'C(0)', 'A(1)', 'B(1)', 'C(1)', 'vo',
+ 'DJ(0)', 'DJ(1)', 'DJK(0)', 'DJK(1)', 'DK(0)', 'DK(1)', 'd1(0)', 'd1(1)',
+ 'd2(0)', 'd2(1)', 'HJ(0)', 'HJ(1)', 'HJK(0)', 'HJK(1)', 'HKJ(0)',
+ 'HKJ(1)', 'HK(0)', 'HK(1)', 'h1(0)', 'h1(1)', 'h2(0)', 'h2(1)', 'h3(0)',
+ 'h3(1)'/
c
      OPEN(UNIT=2, FILE='INPUT.DAT', STATUS='OLD')
      OPEN(UNIT=6, FILE='OUTPUT.DAT', STATUS='NEW')
      first=0
      tnum=0
      CALIB=1.0
      read(2,*) marq,debug,delchi,delgrad
      read(2,*) panum,pred,iter
      read(2,*) rid,rap

      do 10 i1=1,panum
         read(2,*) pa(i1),paf(i1)
10      continue

c      READ IN THE DATA: USE NU greater than 7 to end loop

         temp1=0
         do 30 i1=1,2999
c      nu,nl      upper,lower vibrational state

```



```

c      ju,jl      "      "      J
c      kpu,kpl      "      "      Kp
c      kou,kol      "      "      Ko
40      read(2,*)nu(i1),ju(i1),kpu(i1),kou(i1),
      +nl(i1),jl(i1),kpl(i1),kol(i1),tra(i1),utr(i1),cm(i1)
      if(nu(i1).gt.7)goto70
c      trasforma le frequenze da cm-1 a MHz
if(cm(i1).eq.1) then
      tra(i1)=tra(i1)*29979.2458*CALIB
      endif
tnum=tnum+1
      if (ju(i1).gt.temp1) then
      temp1=ju(i1)
      endif
      if (jl(i1).gt.temp1) then
      temp1=jl(i1)
      endif
30      continue
c
70      if(pred.eq.1)goto80
c
      maxfn=20480
      err=0
c      iter=30
c
      call nllsq(tra,utr,res,tnum,panum,xnum,pa,paf,upa,
1          dbug,marq,chsq,delchi,delgrad,err,grad,
2          iter,alphin,rid,rap)
c
      if(err.ne.0) then
      write(6,*) 'Fit has not converged;err= ',err
      write(6,*)
      endif
      write(6,*)
      write(6,159)
      write(6,*)
159      format(12X,'TRANSITION',17X,'FREQ. EXPERI',5X,'FREQ. CALC.'
      * 3X,'DIFFERENCE')
      do 165 i1=1,tnum
if(cm(i1).eq.1) then
      RES(i1)=RES(i1)/29979.2458
      TRA(i1)=TRA(i1)/29979.2458

```

```

        ENDIF
        write(6,160) i1,nu(i1),ju(i1),kpu(i1),kou(i1),nl(i1),jl(i1)
        +,kpl(i1),kol(i1),tra(i1),res(i1),TRA(I1)-RES(I1)
160      format(' ',i4,2x,i2,2x,i2,2x,i2,2x,i2,2x,i2,2x,i2,2x,i2,2x
        +,i2,2x,f14.5,2x,f14.5,2X,F10.4)
        res(i1)=tra(i1)-res(i1)
sigma=sigma+res(i1)*res(i1)
165      continue
168      continue
        goto 169
        call calA(res,tnum,pa,panum,ifail,rap)
        endif
        write(6,161)
        write(6,*)
161      format(12X,'TRANSITION',17X,'FREQ. EXPERI',5X,'FREQ. CALC.'
        +,3X,'DIFFERENCE')
C
        DO 1001 I=1,TNUM-1
        DO 1002 J=I+1,TNUM
        DIFF=RES(J)-RES(I)
        IF(DIFF.GT.0.0)GOTO 1002
        RESU=RES(I)
        NUU=NU(I)
        NLU=NL(I)
        JUU=JU(I)
        JLU=JL(I)
        KPUU=KPU(I)
        KPLU=KPL(I)
        KOUU=KOU(I)
        KOLU=KOL(I)
        TRAU=TRA(I)
C
        RES(I)=RES(J)
        NU(I)=NU(J)
        NL(I)=NL(J)
        JU(I)=JU(J)
        JL(I)=JL(J)
        KPU(I)=KPU(J)
        KPL(I)=KPL(J)
        KOU(I)=KOU(J)
        KOL(I)=KOL(J)
        TRA(I)=TRA(J)

```

```

C
    RES(J)=RESU
    NU(J)=NUU
    NL(J)=NLU
    JU(J)=JUJ
    JL(J)=JLU
    KPU(J)=KPUU
    KPL(J)=KPLU
    KOU(J)=KOUU
    KOL(J)=KOLU
    TRA(J)=TRAU

C
1002  CONTINUE
1001  CONTINUE
C
C
    do 175 i1=1,tnum
if(cm(i1).eq.1) then
    RES(i1)=RES(i1)/29979.2458
    TRA(i1)=TRA(i1)/29979.2458
    ENDIF
    write(6,162) i1,nu(i1),ju(i1),kpu(i1),kou(i1),nl(i1),jl(i1)
+,kpl(i1),kol(i1),tra(i1),res(i1),tra(i1)-res(i1)
162    format(' ',i4,2x,i2,2x,i2,2x,i2,2x,i2,2x,i2,2x,i2,2x,i2,2x
+,i2,2x,f14.5,2x,f14.5,2x,f10.4)
175    continue

c    OUTPUT CONSTANTS:
c
169    write(6,*)
    write(6,3)
3    format(' *****')
    write(6,*)
    if(rid.eq.'S') then
    write(6,1)
1    format(' REDUCTION SCHEME = S')
    else
    write(6,2)
2    format(' REDUCTION SCHEME = A')
    endif
    write(6,*)
    do 180 i1=1,panum

```

```

c      write (*,170) i1,pname(i1),pa(i1),upa(i1)*dsqrt(chsq)
      write (6,170) i1,pname(i1),pa(i1),upa(i1)*dsqrt(chsq)
170  format(2x,i3,2x,a6,'= ',g25.9,'(',g12.4,')')
180  continue
c
c      OUTPUT CORRELATION MATRIX WITH SCALED DIAGONAL
c
      write(6,*)
      do 190 i1=1,xnum
        write(6,185) (alphin(i1,i2), i2=1,i1)
185   format(40(f4.1,x))
190  continue
rms=sigma/(tnum-XNUM)
rms=dsqrt(rms)
      sigma=dsqrt(chsq)
      write(6,*)

      write(6,*)'rms=',rms,' sigma=',sigma,' chsq=',chsq,
+' grad=',grad,' iter=',iter

      end
c
c      PERFORMS THE LEAST SQUARES FIT
c
      subroutine nllsq(obs,osig,calc,onum,panum,xnum,pa,paf,pasig,
1          dbug,marq,chsq,delchi,delgrad,err,grad,
2          iter,alphin,rid,rap)
c
      integer onum,panum,fnum,err,xnum,xpos(40),paf(40),
1dbug,iter,icount,ifail
      double precision obs(3000),calc(3000),osig(3000),pa(40),
1      pasig(40),marq,chsq,delchi,x(40),
2      nextx(40),alpha(40,40),beta(40),
3      deriv(40,3000),grad,delgrad,ograd,ocalc(3000),
4      alphin(40,40),weight(3000),chold
      character*1 rid
c
c      VARIABLES USED IN PROGRAM
c
c      OBS      ARRAY OF OBSERVED FUNCTION VALUES
c      OSIG     UNCERTAINTIES OF OBSERVABLES
c      CALC     ARRAY OF CALCULATED FUNCT. VALUES

```

c     ONUM         NUMBER OF OBSERVED PARAMETERS  
 c     PANUM        NUMBER OF FITTING PARAMETERS. IT AND ONUM MUST  
 c                   BE EXACTLY THE DIMENSIONS OF OBS AND PA AS DI-  
 c                   MENSIONED IN THE CALLING PROGRAM; DIMENSIONS  
 c                   MAY BE LARGER THAN THE ACTUAL NUMBER OF OBSER-  
 c                   VATIONS AND PARAMETERS AS LONG AS THE EXCESS  
 c                   ONES ARE CONSTRAINED TO ZERO AND THE CORRESPON-  
 c                   DING PAF=0  
 c     PA            ARRAY OF FITTING PARAMETERS  
 c     PAF           FITTING FLAGS;=0 FOR PARAMETERS HELD CONSTANT,  
 c                   =1 FOR FITTED PARAMETERS  
 c     PASIG         ARRAY THAT RETURNS UNCERTAINTIES IN PARAMETERS  
 c     MARQ          MARQUARD PARAMETER; LARGE VALUE INDICATES  
 c                   STEEPEST DESCENT STEP, SMALL VALUE NEWTON  
 c                   (LINEARIZED CHSQ) STEP. SHOULD BE SET TO 0.001  
 c                   INITIALLY  
 c     CHSQ          CHI\*\*2 OF FIT  
 c     DELCHI        IF TWO SUCCESSIVE CHSQ AGREE WITHIN DELCHI, THE  
 c                   FIT IS TERMINATED  
 c     DELGRAD       IF THE GRADIENT OF CHSQ FALLS BELOW DELGRAD, THE  
 c                   FIT IS TERMINATED  
 c     ERR           ERROR CODE;SHOULD BE SET TO ZERO INITIALLY.  
 c                   ERR=1: NO PARAMETERS FITTED;ONLY CHSQ IS RETURNED  
 c                   ERR=2: MORE PARAMETERS THAN OBSERVABLES FITTED  
 c                   ERR=3: MATRIX INVERSION FAILED;JACOBIAN SINGULAR  
 c                   ERR=4: RECOVERY FROM SINGULAR JACOBIAN FAILED  
 c                   ERR=5: NUMBER OF ITERATIONS IN ITER EXCEEDED  
 c                   ERR=6: MARQ EXCEEDED 10\*\*10; SSQ CANNOT BE MINI-  
 c                   MIZED BECAUSE GRADIENTS TOO STEEP OR DELCHI  
 c                   SET UNREALISTICALLY SMALL  
 c                   ERR=7: CAL WAS UNABLE TO COMPUTE ONE OF THE OB-  
 c                   SERVABLES  
 c                   ERR=8: MATRIX INVERSION TO COMPUTE UNCERT. FAILED  
 c     ITER          MAXIMUM NUMBER OF ITERATIONS(CALLS OF DERIVATIVE)  
 c  
 c     THE FOLLOWING PARAMETERS MUST NOT BE SET TO ANYTHING INITIALLY,  
 c     BUT ARE USEFUL FOR DEBUGGING OR ADDITIONAL INFORMATION ABOUT  
 c     THE FIT; DIMENSIONING IS AS FOR OBS AND PA  
 c  
 c     X             ARRAY OF THOSE PA WHICH ARE FITTED  
 c     GRAD          NORM OF THE GRADIENT OF CHSQ;SHOULD BE CLOSE TO  
 c                   ZERO NEAR THE MINIMUM

```

c      NEXTX      ARRAY OF FITTING PARAMETERS BEFORE TESTING FOR
c                  ITS VIABILITY IN DECREASING CHSQ
c      ALPHA      MATRIX THAT CONTAINS THE JACOBIAN TRANSPOSE TIMES
c                  THE JACOBIAN
c      BETA        GRADIENT OF SSQ
c      DERIV       MATRIX OF DERIVATIVES OF ALL OBS W/R TO ALL PARA-
c                  METERS
c
c      DETERMINE CONSTANTS TO BE FIT AND THEIR NUMBER
c
c      icount=0
c      ograd=0d0
c      xnum=0
c      do 10 i1=1,panum
c          if(paf(i1).ne.0) then
c              xnum=xnum+1
c              xpos(xnum)=i1
c              x(xnum)=pa(i1)
c          endif
10      continue
c
c      CALCULATE WEIGHTS
c
c      do 20 i1=1,onum
c          weight(i1)=1d0/(osig(i1)*osig(i1))
20      continue
c
c      if(xnum.eq.0) then
c          call chisq(chsq,obs,calc,weight,onum,pa,panum,x,xnum,
+      xpos,ifail,rid,rap)
c          err=1
c          return
c      endif
c
c      EVALUATE DEGREES OF FREEDOM
c
c      write(*,22)onum
22      format(' number of transitions = ',I5)
c      write(*,23)xnum
23      format(' number of fitted parameters = ',I5)
c      fnum=onum-xnum
c      if (fnum.lt.1) then

```

```

        err=2
        return
    endif

c
c    EVALUATE INITIAL CHSQ; NOTE THAT THIS ALSO CALCULATES
c    CALC FOR THE PARAMETER SET X
c
    call chisq(chold,obs,calc,weight,onum,pa,panum,x,xnum,
+xpos,ifail,rid,rap)
c
c    CALCULATE  $\tilde{(J)} * F * dF/dX$  , THE GRADIENT OF CHSQ AND THE
c     $\tilde{J} * J$  MATRIX, WHERE  $F=(O-C)/OSIG$  AND  $\tilde{\phantom{x}}$  MEANS TRANSPOSE
c
25    do 30 i1=1,xnum
        beta(i1)=0d0
        do 30 i2=1,i1
            alpha(i1,i2)=0d0
30    continue
c
        icount=icount+1
        call der(calc,ocalc,onum,xnum,xpos,panum,pa,deriv,rid,rap)
        do 50 i1=1,onum
            do 40 i2=1,xnum
                beta(i2)=beta(i2)+weight(i1)*(obs(i1)-calc(i1))*
1                deriv(i2,i1)
                do 40 i3=1,i2
                    alpha(i2,i3)=alpha(i2,i3)+weight(i1)*deriv(i2,i1)
1                    *deriv(i3,i1)
40            continue
50        continue
        do 60 i1=1,xnum
            do 60 i2=1,i1
                alpha(i2,i1)=alpha(i1,i2)
60        continue
c
c    CALCULATE PARAMETER INCREMENTS AS  $DELX=BETA*(MARQ*DIAGONAL($ 
c     $ALPHA)+ALPHA)^{-1}$  AND ADD TO X TO GIVE NEXTX, THE NEW TRIAL
c    SET OF PARAMETERS. NOTE THAT A SCALED ALPHA IS INVERTED, TO
c    IMPROVE ACCURACY, AND THEN RESCALED
c
65    do 80 i1=1,xnum
        do 70 i2=1,xnum

```

```

        alphin(i1,i2)=alpha(i1,i2)/dsqrt(alpha(i1,i1)*alpha(i2,i2))
70      continue
        alphin(i1,i1)=1d0+marq
80      continue
        call invert(alphin,xnum,det,err)
        if(err.ne.0) then
            if(err.eq.4) then
                return
            else
                chsq=1.0001d0*chold
                err=4
                go to 95
            endif
        endif
        do 90 i1=1,xnum
            nextx(i1)=x(i1)
            do 90 i2=1,xnum
                nextx(i1)=nextx(i1)+beta(i2)*alphin(i1,i2)/dsqrt(
1                  alpha(i1,i1)*alpha(i2,i2))
90      continue
c
c      CALCULATE NEW TRIAL CHSQ AND CHECK IF IT INCREASED OR DE-
c      CREASED. IF IT DECREASED, NEXTX BECOMES X. SINCE CHSQ HAS
c      ALREADY EVALUATED CALC(NEXTX), THE NEXT ITERATION CAN BE
c      CONTINUED BY CALCULATING A NEW ALPHA AND BETA.
c      IF CHSQ INCREASED, THE MARQUARDT PARAMETER MUST BE INCREA-
c      SED TO FORCE DESCENT IN CHSQ. NEXTX IS DISCARDED AND A
c      SMALLER STEP AWAY FROM THE ORIGINAL X IS TRIED
c
        call chisq(chsq,obs,calc,weight,onum,pa,panum,nextx,
1          xnum,xpos,ifail,rid,rap)
95      if(chold-chsq.gt.0d0.and.ifail.eq.0) then
            grad=0d0
            do 100 i1=1,xnum
                x(i1)=nextx(i1)
                grad=grad+beta(i1)*beta(i1)
100     continue
            grad=dsqrt(grad)
            if(dabs(chold-chsq).lt.delchi.or.dabs(ograd-grad).
1          lt.delgrad) then
                call statist(pasig,xpos,alphin,alpha,xnum)
                return

```



```

endif
marq=marq/10d0
ograd=grad
chold=chsq
if(debug.eq.1) then
  write(6,125) chsq,grad,marq
125   format(' ****/'/'CHI**2= ',e15.7/' PREV.GRAD= ',e15.7/'MARQ= ',
1      e10.2)
  do 140 i1=1,xnum
    write(6,135) i1,x(i1),beta(i1)
135    format(' #',i2,' X= ',e15.8,' PREV.GRAD= ',e15.7)
140    continue
  endif
  go to 25
else if(ifail.ne.0) then
  err=7
  call statist(pasig,xpos,alphin,alpha,xnum)
  return
else
  if(iter.lt.icount) then
    err=5
    call statist(pasig,xpos,alphin,alpha,xnum)
    return
  endif
  marq=max(marq*10d0,0.001d0)
  if(marq.gt.1d10) then
    err=6
    call statist(pasig,xpos,alphin,alpha,xnum)
    return
  endif
  if(debug.eq.1) then
    write(6,145) chsq,grad,marq
145    format(' ****/'/'CHI**2= ',e15.7/' GRAD= ',e15.7/'MARQ= ',
1      e10.2/' ITERATION FAILED')
    do 155 i1=1,xnum
      write(6,150) i1,nextx(i1),beta(i1)
150      format(' #',i2,' NEXTX= ',e15.8,' GRAD= ',e15.7)
155      continue
    endif
    do 160 i1=1,onum
      calc(i1)=ocalc(i1)
160      continue

```

```

        go to 65
    endif
end

c
c  CHISQ RETURNS THE REDUCED CHI**2 AFTER CALLING THE ROUTINE
c  OBSERVED WHICH SHOULD RETURN THE OBSERVED VALUES
c
    subroutine chsq(chsq,obs,calc,weight,onum,pa,
1          panum,x,xnum,xpos,ifail,rid,rap)
c
c  HERE ALSO ODIM AND PADIM MUST BE SET TO THE EXACT DIMENSIONS
c  OF THE ARRAYS IN THE CALLING PROGRAM
c
    double precision chsq,obs(3000),calc(3000),weight(3000),pa(40),
1x(40)
    integer onum,panum,xnum,i1,xpos(40),ifail
    character*1 rid
    do 10 i1=1,xnum
        pa(xpos(i1))=x(i1)
10    continue
    if(rid.eq.'A') then
        call calA(calc,onum,pa,panum,ifail,rap)
    else

    endif
    chsq=0d0
    do 20 i1=1,onum
        chsq=chsq+(obs(i1)-calc(i1))*(obs(i1)-calc(i1))*weight(i1)
20    continue
    chsq=chsq/(onum-xnum)
    return
end

c
c  INVERT COMPUTES THE INVERSE OF MAT AND RETURNS IT AND THE
c  DETERMINANT; IT FIRST THE LARGEST ELEMENTS OF ANY COLUMN
c  ON THE DIAGONAL AND THE DIVIDES AND ADDS TO ZERO THE OTHER
c  ELEMENTS IN THE STANDARD INVERSION ALGORITHM
c
    subroutine invert(mat,dim,det,err)
    double precision mat(40,40),max,save,det
    integer ik(40),jk(40),dim,err
    det=1d0

```

```

do 100 i1=1,dim
  max=0d0
5  do 10 i2=i1,dim
    do 10 i3=i1,dim
      if(dabs(max).le.dabs(mat(i2,i3))) then
        max=mat(i2,i3)
        ik(i1)=i2
        jk(i1)=i3
      endif
10  continue
    if(max.eq.0d0) then
      err=3
      return
    endif
    i2=ik(i1)
    if(i2.gt.i1) then
      do 20 i3=1,dim
        save= mat(i1,i3)
        mat(i1,i3)=mat(i2,i3)
        mat(i2,i3)=--save
20  continue
      endif
      if(i2.ge.i1) then
        i3=jk(i1)
        if(i3.gt.i1) then
          do 30 i2=1,dim
            save=mat(i2,i1)
            mat(i2,i1)=mat(i2,i3)
            mat(i2,i3)=--save
30  continue
          endif
          if(i3.ge.i1) then
            do 40 i2=1,dim
              if(i2.ne.i1) then
                mat(i2,i1)=--mat(i2,i1)/max
              endif
40  continue
            do 50 i2=1,dim
              do 50 i3=1,dim
                if(i1.ne.i2.and.i1.ne.i3) then
                  mat(i2,i3)=mat(i2,i3)+mat(i2,i1)*mat(i1,i3)
                endif
              do 50 i3=1,dim
            do 50 i2=1,dim
          endif
        endif
      endif
    endif
  endif
enddo

```

```

50      continue
      do 60 i3=1,dim
        if(i3.ne.i1) then
          mat(i1,i3)=mat(i1,i3)/max
        endif
60      continue
      mat(i1,i1)=1d0/max
c      det=det*max
      else
        go to 5
      endif
      else
        go to 5
      endif
100    continue
c
c      ORDER MATRIX IN ORIGINAL WAY
c
      do 130 i4=1,dim
        i1=dim-i4+1
        i3=ik(i1)
        if(i3.gt.i1) then
          do 110 i2=1,dim
            save=mat(i2,i1)
            mat(i2,i1)=-mat(i2,i3)
            mat(i2,i3)=save
110        continue
          endif
          i2=jk(i1)
          if(i2.gt.i1) then
            do 120 i3=1,dim
              save=mat(i1,i3)
              mat(i1,i3)=-mat(i2,i3)
              mat(i2,i3)=save
120          continue
            endif
130        continue
      err=0
      return
      end
c
c      DER CALCULATES THE DERIVATIVES OF ALL OBS W/R TO ALL X

```

```

c      IT ALSO SAVES CALC FOR RECOVERY SHOULD SSQ NOT DECREASE
c
      subroutine der(calc,ocalc,onum,xnum,xpos,panum,pa,deriv,rid,rap)
c
c      SET ODIM AND PADIM AGAIN
c
      double precision calc(3000),frac,save,deriv(40,3000),
      localc(3000)

      integer nl(3000),nu(3000),ju(3000),jl(3000),
1  iso(3000),i1,i2,panum,paf(40),enum,temp1,
2  first,ie(3000,5),onum,xpos(40),ifail,xnum
      character*1 rid

      double precision tra(3000),
1  utr(3000),pa(40),e(3000,3),
2  de(3000),b(3000)
      integer kpu(3000),kpl(3000),kou(3000),kol(3000)
      common /obs/tra,nl,nu,ju,jl,utr,de,ie,enum,first,b,paf,iso,
      +kpu,kpl,kou,kol,temp1

do 10 i1=1,onum
      ocalc(i1)=calc(i1)
10  continue
      do 30 i1=1,xnum
          save=pa(xpos(i1))
frac=1d-7
25  pa(xpos(i1))=pa(xpos(i1))*(1.d0+frac)
      if(pa(xpos(i1)).eq.0) then
          pa(xpos(i1))=1d-7
      endif
      if(rid.eq.'A') then

          call calA(calc,onum,pa,panum,ifail,rap)
      else
      endif
      do 20 i2=1,onum
          if(save.ne.0) then
              deriv(i1,i2)=(calc(i2)-ocalc(i2))*1d7/save
else
              deriv(i1,i2)=(calc(i2)-ocalc(i2))*1d7
          endif

```

```

20      continue
      pa(xpos(i1))=save
30      continue
      return
      end

c
c      STATIST EVALUATES UNCERTAINTIES IN PARAMETERS
c
      subroutine statist(pasig,xpos,alphin,alpha,xnum)
      double precision pasig(40),alphin(40,40),alpha(40,40),
1det
      integer xpos(40),i1,xnum,err
      do 50 i1=1,xnum
        do 50 i2=1,xnum
          alphin(i1,i2)=alpha(i1,i2)/dsqrt(alpha(i1,i1)*alpha(i2,i2))
50      continue
      call invert(alphin,xnum,det,err)
      if(err.ne.0) then
        err=8
      endif
      do 80 i1=1,xnum
        pasig(xpos(i1))=dsqrt(alphin(i1,i1)/alpha(i1,i1))
80      continue
      do 100 i1=1,xnum
        do 100 i2=1,xnum
          alphin(i1,i2)=alphin(i1,i2)/dsqrt(alpha(i1,i1)*alpha(i2,i2))/
1          (pasig(xpos(i1))*pasig(xpos(i2)))
100     continue
      return
      end

c

c
c      SUBROUTINE CAL.A. RETURNS CALC FREQUENCIES TO NLLSQ
c
c      Subroutine utilizzata per la riduzione A
c
c      Diagonalization is performed for even and odd k separately because
c      I feel the need for speed.
      subroutine calA(calc,tnum,pa,panum,ifail,rap)
      parameter (np=141)

```

```

integer ii,n,jmax,rap
double precision d(141),z(141,141),wk(2555),pa(40),b(3000)
double precision rx(0:10),ry(0:10),rz(0:10),TRA(3000),utr(3000)
double precision hj(0:10),hjk(0:10),hkj(0:10),hk(0:10)
integer mm,inn,ioo,ipp,qq,rr,ss,tt,uu,vv,paf(40)
integer tnum,nfit(6),enum,ie(3000,5),temp1,mmm,nnn,ppp,qqq,ooo
integer nu(3000),nl(3000),ju(3000),jl(3000),ww,iso(3000)
integer kpu(3000),kou(3000),kpl(3000),kol(3000)
double precision calc(3000),e(3000,3),de(3000),d2(0:10)
double precision ham3(0:1,0:70,0:70,0:70),A(141,141)
double precision hf(-70:70,-70:70),d1(0:10),h2(0:10),h3(0:10)
double precision h1(0:10),nn,oo,pp,dumb,dr(141),dg(141),nz
double precision dj(0:10),hhh(0:10),dk(0:10),xy,xx,yy
common /obs/tra,nl,nu,ju,jl,utr,de,ie,enum,first,b,paf,iso,
+kpu,kpl,kou,kol,temp1
c jmax is the maximum J to be calculated
c ii is the number of vibrational states
    jmax=temp1
    ii=1

c Rotational constants. Scelta del tipo di rappresentazione (Ir opp. III 1)

    if(rap.eq.1) then
        rz(0)=pa(1)
        rx(0)=pa(2)
        ry(0)=pa(3)
        rz(1)=pa(4)
        rx(1)=pa(5)
        ry(1)=pa(6)
    else
        ry(0)=pa(1)
        rx(0)=pa(2)
        rz(0)=pa(3)
        ry(1)=pa(4)
        rx(1)=pa(5)
        rz(1)=pa(6)
    endif
c Band origin is pa(7)
c Quartic distortion constants
    dj(0)=pa(8)
    dj(1)=pa(9)
c hhh is djk

```

```

      hhh(0)=pa(10)
      hhh(1)=pa(11)
      dk(0)=pa(12)
      dk(1)=pa(13)
      d1(0)=pa(14)
      d1(1)=pa(15)
      d2(0)=pa(16)
      d2(1)=pa(17)
c    Sextic distortion constants
      hj(0)=pa(18)
      hj(1)=pa(19)
      hjk(0)=pa(20)
      hjk(1)=pa(21)
      hkj(0)=pa(22)
      hkj(1)=pa(23)
      hk(0)=pa(24)
      hk(1)=pa(25)
      h1(0)=pa(26)
      h1(1)=pa(27)
      h2(0)=pa(28)
      h2(1)=pa(29)
      h3(0)=pa(30)
      h3(1)=pa(31)
c    Calculate matrix elements
      do 220 mm=0,ii
        do 210 nn=1,jmax
          inn=nn
          ioa=1
          do 200 oo=-nn,nn,2
            ioo=oo
            ipa=1
            do 190 pp=-nn,nn,2
              ipp=pp
              if (oo.eq.pp) then
                xx=.5*(rx(mm)+ry(mm))
                yy=xx*(nn*(nn+1)-oo**2)
                xy=.5*(2*oo**2*rz(mm))
                hf(ioo,ipp)=yy+xy
                hf(ioo,ipp)=yy+xy-dj(mm)*(nn*(nn+1))**2-hhh(mm)*
+((nn*(nn+1))*oo**2-dk(mm)*oo**4
++hj(mm)*(nn*(nn+1))**3+hjk(mm)*(nn*(nn+1))**2*oo**2
++hkj(mm)*(nn*(nn+1))*oo**4+hk(mm)*oo**6

```



```

        else
            if (pp.eq.oo+2) then
                hf(ioo,ipp)=(.25*(rx(mm)-ry(mm))-d1(mm)*nn*(nn+1)
+-0.5*d2(mm)*((oo+2)**2+oo**2)+h1(mm)*(nn*(nn+1))**2+
+0.5*h2(mm)*nn*(nn+1)*((oo+2)**2+oo**2)
++0.5*h3(mm)*((oo+2)**4+oo**4))
+*dsqrt((nn*(nn+1)-oo*(oo+1)))*
+dsqrt(nn*(nn+1)-(oo+1)*(oo+2))
            else
                if (pp.eq.oo-2) then
                    hf(ioo,ipp)=(.25*(rx(mm)-ry(mm))-d1(mm)*nn*(nn+1)
+-0.5*d2(mm)*((oo-2)**2+oo**2)+h1(mm)*(nn*(nn+1))**2+
+0.5*h2(mm)*nn*(nn+1)*((oo-2)**2+oo**2)
++0.5*h3(mm)*((oo-2)**4+oo**4))
+*dsqrt((nn*(nn+1)-oo*(oo-1)))*
+dsqrt(nn*(nn+1)-(oo-1)*(oo-2))
                else
                    hf(ioo,ipp)=0
                endif
            endif
        endif
        A(ioa,ipa)=hf(ioo,ipp)
        ipa=ipa+1
190    continue
        ioa=ioa+1
200    continue
        n=nn+1
c    Diagonalize by J
        call TRED2(A,n,np,d,e)
        call TQLI(d,e,n,np,z)
        nz=-nn+1
        ioa=1
        do 202 oo=nz,nn,2
            ioo=oo
            ipa=1
            do 201 pp=nz,nn,2
                ipp=pp
                if (oo.eq.pp) then
                    xx=.5*(rx(mm)+ry(mm))
                    yy=xx*(nn*(nn+1)-oo**2)
                    xy=.5*(2*oo**2*rz(mm))
                    hf(ioo,ipp)=yy+xy

```

```

        hf(ioo,ipp)=yy+xy-dj(mm)*(nn*(nn+1))**2-hhh(mm)*
+(nn*(nn+1))*oo**2-dk(mm)*oo**4
++hj(mm)*(nn*(nn+1))**3+hjk(mm)*(nn*(nn+1))**2*oo**2
++hkj(mm)*(nn*(nn+1))*oo**4+hk(mm)*oo**6
        else
            if (pp.eq.oo+2) then
                hf(ioo,ipp)=(.25*(rx(mm)-ry(mm))-d1(mm)*nn*(nn+1)
+-0.5*d2(mm)*((oo+2)**2+oo**2)+h1(mm)*(nn*(nn+1))**2+
+0.5*h2(mm)*nn*(nn+1)*((oo+2)**2+oo**2)
++0.5*h3(mm)*((oo+2)**4+oo**4))
**dsqrt((nn*(nn+1)-oo*(oo+1)))*
+dsqrt(nn*(nn+1)-(oo+1)*(oo+2))
            else
                if (pp.eq.oo-2) then
                    hf(ioo,ipp)=(.25*(rx(mm)-ry(mm))-d1(mm)*nn*(nn+1)
+-0.5*d2(mm)*((oo-2)**2+oo**2)+h1(mm)*(nn*(nn+1))**2+
+0.5*h2(mm)*nn*(nn+1)*((oo-2)**2+oo**2)
++0.5*h3(mm)*((oo-2)**4+oo**4))
**dsqrt((nn*(nn+1)-oo*(oo-1)))*
+dsqrt(nn*(nn+1)-(oo-1)*(oo-2))
                else
                    hf(ioo,ipp)=0
                endif
            endif
        endif
        A(ioa,ipa)=hf(ioo,ipp)
        ipa=ipa+1
201    continue
        ioa=ioa+1
202    continue
        n=nn
c      Diagonalize by J
        call TRED2(A,n,np,dg,e)
        call TQLI(dg,e,n,np,z)
c      Combine and sort eigenvalues for each J
        do 203 mmm=1,nn+1
            ooo=ooo+1
            dr(ooo)=d(mmm)
c            print *,d(mmm)
203    continue
        do 204 nnn=1,nn
c            print *,dg(nnn)

```

```

        ooo=ooo+1
        dr(ooo)=dg(nnn)
c        print *, '2', inn, ooo, dr(ooo)
204    continue
        ooo=0
        rr=2*inn+1
        do 206 ppp=1,rr
            do 205 qqq=ppp+1,rr
c                print *, 'ppp', ppp, dr(ppp), inn
c                print *, 'qqq', qqq, dr(qqq)
                if (dr(ppp).gt.dr(qqq)) then
c                    print *, '1', ppp, dr(ppp), qqq, dr(qqq)
                    dumb=dr(qqq)
c                    print *, '2', ppp, dr(ppp), qqq, dr(qqq)
                    dr(qqq)=dr(ppp)
c                    print *, '3', ppp, dr(ppp), qqq, dr(qqq)
                    dr(ppp)=dumb
c                    print *, '4', ppp, dr(ppp), qqq, dr(qqq)
                endif
            205    continue
c        print *, inn, ppp, dr(ppp)
        206    continue
c    Correlate energy levels
        do 207 ss=1,rr
            tt=mod((ss+1),2)
            if (tt.eq.0) then
                uu=nn-vv
            endif
            ham3(mm,inn,vv,uu)=dr(ss)
            ham3(0,0,0,0)=0
            if (mm.eq.1) then
                ham3(mm,inn,vv,uu)=pa(7)+ham3(mm,inn,vv,uu)
            endif
            ham3(1,0,0,0)=pa(7)
c        print *, mm, inn, vv, uu, ham3(mm,inn,vv,uu)
            if (tt.eq.0) then
                vv=vv+1
            endif
        207    continue
        vv=0
        uu=0
210    continue

```

```

220  continue
c    Calculate transition frequencies for least squares routine
      do 500 ww=1,tnum
500    calc(ww)=ham3(nu(ww),ju(ww),kpu(ww),kou(ww))-
      +ham3(nl(ww),jl(ww),kpl(ww),kol(ww))
      return
      end

subroutine TRED2(A,N,NP,D,E)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION A(NP,NP),D(NP),E(NP)
IF(N.GT.1)THEN
  DO 18 I=N,2,-1
    L=I-1
    H=0.DO
    SCALE=0.DO
    IF(L.GT.1)THEN
      DO 11 K=1,L
        SCALE=SCALE+ABS(A(I,K))
11      CONTINUE
      IF(SCALE.EQ.0.)THEN
        E(I)=A(I,L)
      ELSE
        DO 12 K=1,L
          A(I,K)=A(I,K)/SCALE
          H=H+A(I,K)**2
12      CONTINUE
        F=A(I,L)
        G=-SIGN(SQRT(H),F)
        E(I)=SCALE*G
        H=H-F*G
        A(I,L)=F-G
        F=0.DO
        DO 15 J=1,L
          A(J,I)=A(I,J)/H
c          G=0.DO
          DO 13 K=1,J
            G=G+A(J,K)*A(I,K)
13          CONTINUE
          IF(L.GT.J)THEN
            DO 14 K=J+1,L
              G=G+A(K,J)*A(I,K)

```

```

14             CONTINUE
               ENDIF
               E(J)=G/H
               F=F+E(J)*A(I,J)
15             CONTINUE
               HH=F/(H+H)
               DO 17 J=1,L
                 F=A(I,J)
                 G=E(J)-HH*F
                 E(J)=G
                 DO 16 K=1,J
                   A(J,K)=A(J,K)-F*E(K)-G*A(I,K)
16             CONTINUE
17             CONTINUE
               ENDIF
               ELSE
                 E(I)=A(I,L)
               ENDIF
               D(I)=H
18             CONTINUE
ENDIF
c             D(1)=0.DO
             E(1)=0.DO
             DO 23 I=1,N
c               L=I-1
c               IF(D(I).NE.0.)THEN
c                 DO 21 J=1,L
c                   G=0.DO
c                   DO 19 K=1,L
c                     G=G+A(I,K)*A(K,J)
c19                CONTINUE
c                   DO 20 K=1,L
c                     A(K,J)=A(K,J)-G*A(K,I)
c20                CONTINUE
c21                CONTINUE
c               ENDIF
               D(I)=A(I,I)
c               A(I,I)=1.
c               IF(L.GE.1)THEN
c                 DO 22 J=1,L
c                   A(I,J)=0.DO
c                   A(J,I)=0.DO

```

```

c22      CONTINUE
c        ENDIF
23      CONTINUE
        RETURN
        END

subroutine TQLI(D,E,N,NP,Z)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION D(NP),E(NP),Z(NP,NP)
IF (N.GT.1) THEN
  DO 11 I=2,N
    E(I-1)=E(I)
11  CONTINUE
    E(N)=0.DO
    DO 15 L=1,N
      ITER=0
1    DO 12 M=L,N-1
      DD=ABS(D(M))+ABS(D(M+1))
      IF (ABS(E(M))+DD.EQ.DD) GO TO 2
12   CONTINUE
      M=N
2    IF(M.NE.L)THEN
      IF(ITER.EQ.30)PAUSE 'too many iterations'
      ITER=ITER+1
      G=(D(L+1)-D(L))/(2.*E(L))
      R=SQRT(G**2+1.)
      G=D(M)-D(L)+E(L)/(G+SIGN(R,G))
      S=1.DO
      C=1.DO
      P=0.DO
      DO 14 I=M-1,L,-1
        F=S*E(I)
        B=C*E(I)
        IF(ABS(F).GE.ABS(G))THEN
          C=G/F
          R=SQRT(C**2+1.)
          E(I+1)=F*R
          S=1./R
          C=C*S
        ELSE
          S=F/G
          R=SQRT(S**2+1.)

```

```

        E(I+1)=G*R
        C=1./R
        S=S*C
    ENDIF
    G=D(I+1)-P
    R=(D(I)-G)*S+2.*C*B
    P=S*R
    D(I+1)=G+P
    G=C*R-B
c      DO 13 K=1,N
c          F=Z(K,I+1)
c          Z(K,I+1)=S*Z(K,I)+C*F
c          Z(K,I)=C*Z(K,I)-S*F
c13     CONTINUE
14      CONTINUE
        D(L)=D(L)-P
        E(L)=G
        E(M)=0.DO
        GO TO 1
    ENDIF
15      CONTINUE
    ENDIF
    RETURN
    END

```

## Appendix B. Assigned BrNO Spectral Lines

### B.1 Notation

Table B.1 Notation used in lists of assigned lines

N	Line number, in order of increasing wavenumber
$v'$	Upper vibrational level
$J'$	Upper level J
$K'_a$	Upper level $K_a$
$K'_c$	Upper level $K_c$
$v''$	Lower vibrational level
$J''$	Lower level J
$K''_a$	Lower level $K_a$
$K''_c$	Lower level $K_c$
Obs	Observed line position ( $\text{cm}^{-1}$ )
Pred	Predicted line position ( $\text{cm}^{-1}$ )
Diff	Observed - Predicted ( $\text{cm}^{-1}$ )

### B.2 $^{79}\text{BrNO } 2\nu_1$

N	$v'$	$J'$	$K'_a$	$K'_c$	$v''$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	62	8	54	0	63	8	55	3548.9517	3548.95243	-0.0007
2	1	62	8	54	0	63	8	55	3548.9525	3548.95243	0.0001
3	1	61	8	53	0	62	8	54	3549.0763	3549.07678	-0.0005
4	1	61	8	53	0	62	8	54	3549.0769	3549.07678	0.0001
5	1	60	8	52	0	61	8	53	3549.2026	3549.20309	-0.0005
6	1	60	8	52	0	61	8	53	3549.2033	3549.20309	0.0002
7	1	59	8	51	0	60	8	52	3549.3308	3549.33135	-0.0006
8	1	59	8	51	0	60	8	52	3549.3324	3549.33135	0.001
9	1	58	8	50	0	59	8	51	3549.4617	3549.46157	0.0001
10	1	58	8	50	0	59	8	51	3549.4619	3549.46157	0.0003
11	1	57	8	49	0	58	8	50	3549.5932	3549.59375	-0.0005
12	1	57	8	49	0	58	8	50	3549.5933	3549.59375	-0.0004
13	1	63	7	56	0	64	7	57	3549.6177	3549.61758	0.0001
14	1	63	7	56	0	64	7	57	3549.6181	3549.61758	0.0005
15	1	56	8	48	0	57	8	49	3549.7276	3549.72788	-0.0003
16	1	56	8	48	0	57	8	49	3549.7286	3549.72788	0.0007
17	1	62	7	55	0	63	7	56	3549.7397	3549.73986	-0.0002
18	1	62	7	55	0	63	7	56	3549.7398	3549.73986	-0.0001



19	1	55	8	47	0	56	8	48	3549.8633	3549.86397	-0.0007
20	1	61	7	54	0	62	7	55	3549.8637	3549.8641	-0.0004
21	1	55	8	47	0	56	8	48	3549.8638	3549.86397	-0.0002
22	1	60	7	53	0	61	7	54	3549.9907	3549.9903	0.0004
23	1	60	7	53	0	61	7	54	3549.9911	3549.9903	0.0008
24	1	54	8	46	0	55	8	47	3550.0023	3550.00202	0.0003
25	1	54	8	46	0	55	8	47	3550.0025	3550.00202	0.0005
26	1	59	7	52	0	60	7	53	3550.1178	3550.11846	-0.0007
27	1	59	7	52	0	60	7	53	3550.1182	3550.11846	-0.0003
28	1	53	8	45	0	54	8	46	3550.1413	3550.14203	-0.0007
29	1	53	8	45	0	54	8	46	3550.1424	3550.14203	0.0004
30	1	58	7	51	0	59	7	52	3550.248	3550.24858	-0.0006
31	1	58	7	51	0	59	7	52	3550.2491	3550.24858	0.0005
32	1	52	8	44	0	53	8	45	3550.2836	3550.28399	-0.0004
33	1	52	8	44	0	53	8	45	3550.284	3550.28399	0
34	1	57	7	50	0	58	7	51	3550.3806	3550.38066	-0.0001
35	1	57	7	50	0	58	7	51	3550.3811	3550.38066	0.0004
36	1	51	8	43	0	52	8	44	3550.4272	3550.42792	-0.0007
37	1	51	8	43	0	52	8	44	3550.428	3550.42792	0.0001
38	1	56	7	49	0	57	7	50	3550.514	3550.5147	-0.0007
39	1	56	7	49	0	57	7	50	3550.5147	3550.5147	0
40	1	61	6	55	0	62	6	56	3550.5494	3550.54914	0.0003
41	1	50	8	42	0	51	8	43	3550.5737	3550.5738	-0.0001
42	1	50	8	42	0	51	8	43	3550.5743	3550.5738	0.0005
43	1	55	7	48	0	56	7	49	3550.6498	3550.6507	-0.0009
44	1	55	7	48	0	56	7	49	3550.65	3550.6507	-0.0007
45	1	69	4	66	0	70	4	67	3550.6739	3550.67447	-0.0006
46	1	69	4	65	0	70	4	66	3550.68	3550.67964	0.0004
47	1	49	8	41	0	50	8	42	3550.7211	3550.72164	-0.0005
48	1	49	8	41	0	50	8	42	3550.7216	3550.72164	0
49	1	68	4	65	0	69	4	66	3550.7848	3550.78437	0.0004
50	1	54	7	47	0	55	7	48	3550.7881	3550.78866	-0.0006
51	1	68	4	64	0	69	4	65	3550.7882	3550.7889	-0.0007
52	1	54	7	47	0	55	7	48	3550.789	3550.78866	0.0003
53	1	48	8	40	0	49	8	41	3550.8705	3550.87144	-0.0009
54	1	48	8	40	0	49	8	41	3550.8705	3550.87144	-0.0009
55	1	67	4	64	0	68	4	65	3550.8958	3550.89624	-0.0004
56	1	67	4	63	0	68	4	64	3550.8996	3550.90019	-0.0006
57	1	53	7	46	0	54	7	47	3550.9284	3550.92858	-0.0002
58	1	53	7	46	0	54	7	47	3550.9293	3550.92858	0.0007
59	1	58	6	52	0	59	6	53	3550.9332	3550.93325	0
60	1	66	4	63	0	67	4	64	3551.0101	3551.01009	0
61	1	66	4	62	0	67	4	63	3551.0128	3551.01352	-0.0007
62	1	66	4	62	0	67	4	63	3551.0136	3551.01352	0.0001
63	1	47	8	39	0	48	8	40	3551.0241	3551.0232	0.0009

64	1	47	8	39	0	48	8	40	3551.0243	3551.0232	0.0011
65	1	57	6	51	0	58	6	52	3551.0658	3551.06522	0.0006
66	1	52	7	45	0	53	7	46	3551.07	3551.07047	-0.0005
67	1	52	7	45	0	53	7	46	3551.0713	3551.07047	0.0008
68	1	65	4	62	0	66	4	63	3551.1252	3551.12591	-0.0007
69	1	65	4	61	0	66	4	62	3551.1284	3551.12888	-0.0005
70	1	46	8	38	0	47	8	39	3551.1764	3551.17691	-0.0005
71	1	46	8	38	0	47	8	39	3551.1774	3551.17691	0.0005
72	1	56	6	50	0	57	6	51	3551.2	3551.19915	0.0009
73	1	51	7	44	0	52	7	45	3551.2148	3551.21431	0.0005
74	1	51	7	44	0	52	7	45	3551.2149	3551.21431	0.0006
75	1	64	4	61	0	65	4	62	3551.2441	3551.2437	0.0004
76	1	64	4	60	0	65	4	61	3551.2458	3551.24627	-0.0005
77	1	60	5	55	0	61	5	56	3551.2579	3551.25703	0.0009
78	1	45	8	37	0	46	8	38	3551.3318	3551.33258	-0.0008
79	1	45	8	37	0	46	8	38	3551.332	3551.33258	-0.0006
80	1	55	6	49	0	56	6	50	3551.3354	3551.33505	0.0004
81	1	50	7	43	0	51	7	44	3551.3594	3551.36012	-0.0007
82	1	50	7	43	0	51	7	44	3551.3604	3551.36012	0.0003
83	1	63	4	60	0	64	4	61	3551.3629	3551.36348	-0.0006
84	1	63	4	59	0	64	4	60	3551.3666	3551.36568	0.0009
85	1	59	5	54	0	60	5	55	3551.3848	3551.38489	-0.0001
86	1	69	1	68	0	70	1	69	3551.4066	3551.40617	0.0004
87	1	66	3	63	0	67	3	64	3551.4087	3551.40798	0.0007
88	1	69	1	69	0	70	1	70	3551.4169	3551.41615	0.0008
89	1	69	0	69	0	70	0	70	3551.4318	3551.43179	0
90	1	68	2	66	0	69	2	67	3551.4563	3551.45523	0.0011
91	1	54	6	48	0	55	6	49	3551.4731	3551.47291	0.0002
92	1	62	4	59	0	63	4	60	3551.4848	3551.48523	-0.0004
93	1	62	4	58	0	63	4	59	3551.4868	3551.48712	-0.0003
94	1	44	8	36	0	45	8	37	3551.4899	3551.49022	-0.0003
95	1	44	8	36	0	45	8	37	3551.4905	3551.49022	0.0003
96	1	67	2	66	0	68	2	67	3551.4983	3551.49852	-0.0002
97	1	49	7	42	0	50	7	43	3551.508	3551.50788	0.0001
98	1	49	7	42	0	50	7	43	3551.5085	3551.50788	0.0006
99	1	58	5	53	0	59	5	54	3551.5149	3551.51473	0.0002
100	1	68	1	67	0	69	1	68	3551.5202	3551.51994	0.0003
101	1	65	3	62	0	66	3	63	3551.5207	3551.52114	-0.0004
102	1	68	1	68	0	69	1	69	3551.5322	3551.53208	0.0001
103	1	68	0	68	0	69	0	69	3551.548	3551.54826	-0.0003
104	1	67	2	65	0	68	2	66	3551.5645	3551.56527	-0.0008
105	1	61	4	58	0	62	4	59	3551.6085	3551.60896	-0.0005
106	1	61	4	57	0	62	4	58	3551.6108	3551.61057	0.0002
107	1	53	6	47	0	54	6	48	3551.6131	3551.61274	0.0004
108	1	66	2	65	0	67	2	66	3551.6162	3551.61541	0.0008

109	1	67	1	66	0	68	1	67	3551.6358	3551.63538	0.0004
110	1	64	3	61	0	65	3	62	3551.6361	3551.63645	-0.0003
111	1	57	5	52	0	58	5	53	3551.6465	3551.64654	0
112	1	67	1	67	0	68	1	68	3551.649	3551.64978	-0.0008
113	1	43	8	35	0	44	8	36	3551.6502	3551.64981	0.0004
114	1	48	7	41	0	49	7	42	3551.6579	3551.65761	0.0003
115	1	48	7	41	0	49	7	42	3551.6583	3551.65761	0.0007
116	1	67	0	67	0	68	0	68	3551.6656	3551.66652	-0.0009
117	1	66	2	64	0	67	2	65	3551.6774	3551.67721	0.0002
118	1	65	2	64	0	66	2	65	3551.7343	3551.73412	0.0002
119	1	60	4	57	0	61	4	58	3551.7346	3551.73467	-0.0001
120	1	60	4	56	0	61	4	57	3551.736	3551.73603	0
121	1	52	6	46	0	53	6	47	3551.7537	3551.75453	-0.0008
122	1	63	3	60	0	64	3	61	3551.7546	3551.7539	0.0007
123	1	66	1	66	0	67	1	67	3551.7691	3551.76926	-0.0002
124	1	56	5	51	0	57	5	52	3551.781	3551.78033	0.0007
125	1	66	0	66	0	67	0	67	3551.7867	3551.78654	0.0002
126	1	65	2	63	0	66	2	64	3551.7911	3551.79108	0
127	1	47	7	40	0	48	7	41	3551.8098	3551.80929	0.0005
128	1	47	7	40	0	48	7	41	3551.8101	3551.80929	0.0008
129	1	42	8	34	0	43	8	35	3551.8103	3551.81135	-0.0011
130	1	42	8	34	0	43	8	35	3551.8109	3551.81135	-0.0005
131	1	64	2	63	0	65	2	64	3551.8538	3551.85464	-0.0008
132	1	59	4	56	0	60	4	57	3551.863	3551.86235	0.0006
133	1	59	4	55	0	60	4	56	3551.8635	3551.86351	0
134	1	65	1	64	0	66	1	65	3551.8709	3551.87134	-0.0004
135	1	62	3	59	0	63	3	60	3551.8743	3551.87349	0.0008
136	1	65	1	65	0	66	1	66	3551.8913	3551.89052	0.0008
137	1	51	6	45	0	52	6	46	3551.8973	3551.89829	-0.001
138	1	64	2	62	0	65	2	63	3551.9072	3551.90688	0.0003
139	1	65	0	65	0	66	0	66	3551.9088	3551.90834	0.0005
140	1	55	5	50	0	56	5	51	3551.9159	3551.91609	-0.0002
141	1	41	8	33	0	42	8	34	3551.9741	3551.97486	-0.0008
142	1	41	8	33	0	42	8	34	3551.9748	3551.97486	-0.0001
143	1	63	2	62	0	64	2	63	3551.9767	3551.97699	-0.0003
144	1	61	3	59	0	62	3	60	3551.9783	3551.97736	0.0009
145	1	58	4	55	0	59	4	56	3551.991	3551.99202	-0.001
146	1	58	4	54	0	59	4	55	3551.9929	3551.99299	-0.0001
147	1	61	3	58	0	62	3	59	3551.9954	3551.99522	0.0002
148	1	64	1	64	0	65	1	65	3552.0138	3552.01355	0.0002
149	1	63	2	61	0	64	2	62	3552.0248	3552.02462	0.0002
150	1	64	0	64	0	65	0	65	3552.0318	3552.03192	-0.0001
151	1	54	5	49	0	55	5	50	3552.0542	3552.05382	0.0004
152	1	62	2	61	0	63	2	62	3552.1006	3552.10116	-0.0006
153	1	60	3	58	0	61	3	59	3552.1035	3552.10342	0.0001

154	1	63	1	62	0	64	1	63	3552.1133	3552.11412	-0.0008
155	1	60	3	57	0	61	3	58	3552.1187	3552.11907	-0.0004
156	1	57	4	54	0	58	4	55	3552.1234	3552.12367	-0.0003
157	1	57	4	53	0	58	4	54	3552.1237	3552.12447	-0.0008
158	1	63	1	63	0	64	1	64	3552.138	3552.13836	-0.0004
159	1	40	8	32	0	41	8	33	3552.1412	3552.14032	0.0009
160	1	40	8	32	0	41	8	33	3552.1412	3552.14032	0.0009
161	1	62	2	60	0	63	2	61	3552.1449	3552.14431	0.0006
162	1	63	0	63	0	64	0	64	3552.158	3552.15727	0.0007
163	1	53	5	48	0	54	5	49	3552.1934	3552.19353	-0.0001
164	1	61	2	60	0	62	2	61	3552.228	3552.22717	0.0008
165	1	59	3	57	0	60	3	58	3552.2323	3552.23142	0.0009
166	1	62	1	61	0	63	1	62	3552.2376	3552.23809	-0.0005
167	1	59	3	56	0	60	3	57	3552.2459	3552.24505	0.0008
168	1	56	4	53	0	57	4	54	3552.2577	3552.2573	0.0004
169	1	56	4	52	0	57	4	53	3552.2578	3552.25796	-0.0002
170	1	62	1	62	0	63	1	63	3552.2648	3552.26496	-0.0002
171	1	61	2	59	0	62	2	60	3552.2668	3552.26597	0.0008
172	1	62	0	62	0	63	0	63	3552.2838	3552.28439	-0.0006
173	1	39	8	31	0	40	8	32	3552.3068	3552.30773	-0.0009
174	1	39	8	31	0	40	8	32	3552.3077	3552.30773	0
175	1	52	5	47	0	53	5	48	3552.3352	3552.33521	0
176	1	60	2	59	0	61	2	60	3552.3544	3552.355	-0.0006
177	1	58	3	56	0	59	3	57	3552.3619	3552.36135	0.0006
178	1	61	1	60	0	62	1	61	3552.3631	3552.36379	-0.0007
179	1	58	3	55	0	59	3	56	3552.3724	3552.37316	-0.0008
180	1	60	2	58	0	61	2	59	3552.3887	3552.3896	-0.0009
181	1	55	4	52	0	56	4	53	3552.3933	3552.39291	0.0004
182	1	61	1	61	0	62	1	62	3552.3938	3552.39334	0.0005
183	1	55	4	51	0	56	4	52	3552.3943	3552.39345	0.0008
184	1	61	0	61	0	62	0	62	3552.4143	3552.41329	0.001
185	1	38	8	30	0	39	8	31	3552.4776	3552.4771	0.0005
186	1	51	5	46	0	52	5	47	3552.4781	3552.47886	-0.0008
187	1	59	2	58	0	60	2	59	3552.4845	3552.48468	-0.0002
188	1	60	1	59	0	61	1	60	3552.492	3552.49123	0.0008
189	1	57	3	55	0	58	3	56	3552.4926	3552.49322	-0.0006
190	1	57	3	54	0	58	3	55	3552.5042	3552.50337	0.0008
191	1	59	2	57	0	60	2	58	3552.5144	3552.51522	-0.0008
192	1	60	1	60	0	61	1	61	3552.5233	3552.5235	-0.0002
193	1	54	4	51	0	55	4	52	3552.5296	3552.53049	-0.0009
194	1	54	4	50	0	55	4	51	3552.5318	3552.53094	0.0009
195	1	60	0	60	0	61	0	61	3552.5435	3552.54395	-0.0005
196	1	58	2	57	0	59	2	58	3552.6174	3552.61621	0.0012
197	1	59	1	58	0	60	1	59	3552.6208	3552.62044	0.0004
198	1	50	5	45	0	51	5	46	3552.6238	3552.62449	-0.0007

199	1	50	5	45	0	51	5	46	3552.625	3552.62449	0.0005
200	1	56	3	54	0	57	3	55	3552.6269	3552.62704	-0.0001
201	1	56	3	53	0	57	3	54	3552.636	3552.6357	0.0003
202	1	58	2	56	0	59	2	57	3552.6419	3552.64284	-0.0009
203	1	59	1	59	0	60	1	60	3552.6554	3552.65545	0
204	1	53	4	50	0	54	4	51	3552.6693	3552.67006	-0.0008
205	1	53	4	49	0	54	4	50	3552.6704	3552.67042	0
206	1	59	0	59	0	60	0	60	3552.6756	3552.67638	-0.0008
207	1	58	1	57	0	59	1	58	3552.7506	3552.75141	-0.0008
208	1	57	2	56	0	58	2	57	3552.7508	3552.74958	0.0012
209	1	55	3	53	0	56	3	54	3552.762	3552.76281	-0.0008
210	1	55	3	52	0	56	3	53	3552.7707	3552.77012	0.0006
211	1	57	2	55	0	58	2	56	3552.7721	3552.77246	-0.0004
212	1	49	5	44	0	50	5	45	3552.7721	3552.77208	0
213	1	58	1	58	0	59	1	59	3552.7898	3552.78918	0.0006
214	1	58	0	58	0	59	0	59	3552.8104	3552.81058	-0.0002
215	1	52	4	49	0	53	4	50	3552.8112	3552.81161	-0.0004
216	1	52	4	48	0	53	4	49	3552.8123	3552.81189	0.0004
217	1	56	2	55	0	57	2	56	3552.8839	3552.8848	-0.0009
218	1	57	1	56	0	58	1	57	3552.8844	3552.88415	0.0002
219	1	54	3	52	0	55	3	53	3552.9005	3552.90053	0
220	1	56	2	54	0	57	2	55	3552.9041	3552.90409	0
221	1	54	3	51	0	55	3	52	3552.9071	3552.90663	0.0005
222	1	48	5	43	0	49	5	44	3552.9213	3552.92164	-0.0003
223	1	57	1	57	0	58	1	58	3552.9246	3552.92471	-0.0001
224	1	57	0	57	0	58	0	58	3552.9457	3552.94655	-0.0009
225	1	51	4	47	0	52	4	48	3552.9552	3552.95536	-0.0002
226	1	56	1	55	0	57	1	56	3553.0182	3553.01869	-0.0005
227	1	55	2	54	0	56	2	55	3553.0215	3553.02188	-0.0004
228	1	55	2	53	0	56	2	54	3553.0377	3553.03774	0
229	1	53	3	51	0	54	3	52	3553.0404	3553.0402	0.0002
230	1	53	3	50	0	54	3	51	3553.0445	3553.04524	-0.0007
231	1	56	1	56	0	57	1	57	3553.0613	3553.06202	-0.0007
232	1	47	5	42	0	48	5	43	3553.0723	3553.07317	-0.0009
233	1	56	0	56	0	57	0	57	3553.0845	3553.08428	0.0002
234	1	50	4	46	0	51	4	47	3553.1014	3553.10081	0.0006
235	1	55	1	54	0	56	1	55	3553.1546	3553.15504	-0.0004
236	1	54	2	53	0	55	2	54	3553.1619	3553.16082	0.0011
237	1	54	2	52	0	55	2	53	3553.1725	3553.17342	-0.0009
238	1	52	3	50	0	53	3	51	3553.1822	3553.18183	0.0004
239	1	52	3	49	0	53	3	50	3553.1852	3553.18592	-0.0007
240	1	55	1	55	0	56	1	56	3553.2019	3553.20113	0.0008
241	1	55	0	55	0	56	0	56	3553.2241	3553.22378	0.0003
242	1	46	5	41	0	47	5	42	3553.2265	3553.22667	-0.0002
243	1	49	4	45	0	50	4	46	3553.2486	3553.24825	0.0004

244	1	54	1	53	0	55	1	54	3553.294	3553.29319	0.0008
245	1	53	2	52	0	54	2	53	3553.3012	3553.30163	-0.0004
246	1	53	2	51	0	54	2	52	3553.311	3553.31114	-0.0001
247	1	51	3	49	0	52	3	50	3553.325	3553.32542	-0.0004
248	1	51	3	48	0	52	3	49	3553.3288	3553.32867	0.0001
249	1	54	1	54	0	55	1	55	3553.3422	3553.34203	0.0002
250	1	54	0	54	0	55	0	55	3553.365	3553.36504	0
251	1	48	4	44	0	49	4	45	3553.397	3553.39767	-0.0007
252	1	53	1	52	0	54	1	53	3553.4332	3553.43318	0
253	1	52	2	51	0	53	2	52	3553.4435	3553.44431	-0.0008
254	1	52	2	50	0	53	2	51	3553.4502	3553.45091	-0.0007
255	1	50	3	48	0	51	3	49	3553.4708	3553.47096	-0.0002
256	1	50	3	47	0	51	3	48	3553.4736	3553.47349	0.0001
257	1	53	1	53	0	54	1	54	3553.4838	3553.48473	-0.0009
258	1	53	0	53	0	54	0	54	3553.5073	3553.50807	-0.0008
259	1	47	4	43	0	48	4	44	3553.5499	3553.54907	0.0008
260	1	52	1	51	0	53	1	52	3553.5751	3553.575	0.0001
261	1	51	2	50	0	52	2	51	3553.5886	3553.58886	-0.0003
262	1	51	2	49	0	52	2	50	3553.5919	3553.59272	-0.0008
263	1	49	3	47	0	50	3	48	3553.6181	3553.61847	-0.0004
264	1	49	3	46	0	50	3	47	3553.6194	3553.62037	-0.001
265	1	52	1	52	0	53	1	53	3553.6294	3553.62922	0.0002
266	1	52	0	52	0	53	0	53	3553.6538	3553.65285	0.0009
267	1	46	4	42	0	47	4	43	3553.7034	3553.70246	0.0009
268	1	51	1	50	0	52	1	51	3553.7179	3553.71868	-0.0008
269	1	50	2	49	0	51	2	50	3553.7344	3553.73529	-0.0009
270	1	50	2	48	0	51	2	49	3553.7373	3553.7366	0.0007
271	1	48	3	46	0	49	3	47	3553.7679	3553.76793	0
272	1	48	3	45	0	49	3	46	3553.7689	3553.76929	-0.0004
273	1	48	3	45	0	49	3	46	3553.7699	3553.76929	0.0006
274	1	51	1	51	0	52	1	52	3553.7761	3553.77552	0.0006
275	1	51	0	51	0	52	0	52	3553.7992	3553.7994	-0.0002
276	1	45	4	41	0	46	4	42	3553.8578	3553.85782	0
277	1	42	5	37	0	43	5	38	3553.8606	3553.86034	0.0003
278	1	50	1	49	0	51	1	50	3553.8648	3553.86422	0.0006
279	1	49	2	47	0	50	2	48	3553.8818	3553.88254	-0.0007
280	1	49	2	48	0	50	2	49	3553.884	3553.8836	0.0004
281	1	47	3	44	0	48	3	45	3553.9194	3553.92026	-0.0009
282	1	47	3	45	0	48	3	46	3553.9204	3553.91937	0.001
283	1	50	1	50	0	51	1	51	3553.9236	3553.92362	0
284	1	50	0	50	0	51	0	51	3553.9476	3553.9477	-0.0001
285	1	49	1	48	0	50	1	49	3554.0118	3554.01163	0.0002
286	1	44	4	40	0	45	4	41	3554.0148	3554.01516	-0.0004
287	1	41	5	36	0	42	5	37	3554.0234	3554.02367	-0.0003
288	1	48	2	46	0	49	2	47	3554.0303	3554.03055	-0.0002

289	1	48	2	47	0	49	2	48	3554.0331	3554.03379	-0.0007
290	1	46	3	44	0	47	3	45	3554.0724	3554.07276	-0.0004
291	1	46	3	43	0	47	3	44	3554.0727	3554.07327	-0.0006
292	1	49	1	49	0	50	1	50	3554.0735	3554.07352	0
293	1	49	0	49	0	50	0	50	3554.0975	3554.09777	-0.0003
294	1	48	1	47	0	49	1	48	3554.1618	3554.16092	0.0009
295	1	43	4	39	0	44	4	40	3554.1736	3554.17448	-0.0009
296	1	47	2	45	0	48	2	46	3554.1813	3554.18063	0.0007
297	1	47	2	46	0	48	2	47	3554.1855	3554.18588	-0.0004
298	1	40	5	35	0	41	5	36	3554.1898	3554.18896	0.0008
299	1	48	1	48	0	49	1	49	3554.2251	3554.22523	-0.0001
300	1	45	3	42	0	46	3	43	3554.2278	3554.22831	-0.0005
301	1	45	3	43	0	46	3	44	3554.2289	3554.22812	0.0008
302	1	48	0	48	0	49	0	49	3554.2491	3554.2496	-0.0005
303	1	36	6	30	0	37	6	31	3554.2896	3554.29017	-0.0006
304	1	47	1	46	0	48	1	47	3554.3117	3554.31211	-0.0004
305	1	46	2	44	0	47	2	45	3554.3336	3554.33279	0.0008
306	1	42	4	38	0	43	4	39	3554.3355	3554.33577	-0.0003
307	1	46	2	45	0	47	2	46	3554.3399	3554.33986	0
308	1	39	5	34	0	40	5	35	3554.3573	3554.35621	0.0011
309	1	47	1	47	0	48	1	48	3554.3792	3554.37875	0.0005
310	1	44	3	41	0	45	3	42	3554.3845	3554.38537	-0.0009
311	1	44	3	42	0	45	3	43	3554.3856	3554.38545	0.0001
312	1	47	0	47	0	48	0	48	3554.4028	3554.40319	-0.0004
313	1	35	6	29	0	36	6	30	3554.4644	3554.46531	-0.0009
314	1	46	1	45	0	47	1	46	3554.4655	3554.46521	0.0003
315	1	45	2	43	0	46	2	44	3554.4868	3554.48702	-0.0002
316	1	45	2	44	0	46	2	45	3554.4965	3554.49573	0.0008
317	1	41	4	37	0	42	4	38	3554.4999	3554.49903	0.0009
318	1	38	5	33	0	39	5	34	3554.5245	3554.52543	-0.0009
319	1	46	1	46	0	47	1	47	3554.5347	3554.53407	0.0006
320	1	43	3	40	0	44	3	41	3554.5442	3554.54445	-0.0003
321	1	43	3	41	0	44	3	42	3554.5454	3554.54475	0.0007
322	1	46	0	46	0	47	0	47	3554.5577	3554.55855	-0.0008
323	1	45	1	44	0	46	1	45	3554.6206	3554.62021	0.0004
324	1	34	6	28	0	35	6	29	3554.6417	3554.6424	-0.0007
325	1	44	2	42	0	45	2	43	3554.6437	3554.64334	0.0004
326	1	44	2	43	0	45	2	44	3554.6541	3554.65351	0.0006
327	1	40	4	36	0	41	4	37	3554.6637	3554.66426	-0.0006
328	1	45	1	45	0	46	1	46	3554.6908	3554.69121	-0.0004
329	1	37	5	32	0	38	5	33	3554.6959	3554.69661	-0.0007
330	1	42	3	40	0	43	3	41	3554.7053	3554.70601	-0.0007
331	1	42	3	39	0	43	3	40	3554.7062	3554.70555	0.0007
332	1	45	0	45	0	46	0	46	3554.7158	3554.71567	0.0001
333	1	44	1	43	0	45	1	44	3554.7764	3554.77715	-0.0007

334	1	43	2	41	0	44	2	42	3554.8026	3554.80174	0.0009
335	1	43	2	42	0	44	2	43	3554.8129	3554.81318	-0.0003
336	1	33	6	27	0	34	6	28	3554.8219	3554.82144	0.0005
337	1	39	4	35	0	40	4	36	3554.8321	3554.83146	0.0006
338	1	44	1	44	0	45	1	45	3554.8508	3554.85017	0.0006
339	1	41	3	38	0	42	3	39	3554.8693	3554.86865	0.0006
340	1	41	3	39	0	42	3	40	3554.8698	3554.86924	0.0006
341	1	36	5	31	0	37	5	32	3554.8706	3554.86974	0.0009
342	1	44	0	44	0	45	0	45	3554.8738	3554.87456	-0.0008
343	1	43	1	42	0	44	1	43	3554.9364	3554.93601	0.0004
344	1	42	2	40	0	43	2	41	3554.9613	3554.96222	-0.0009
345	1	42	2	41	0	43	2	42	3554.9747	3554.97477	-0.0001
346	1	38	4	34	0	39	4	35	3555.0005	3555.00063	-0.0001
347	1	32	6	26	0	33	6	27	3555.0013	3555.00244	-0.0011
348	1	43	1	43	0	44	1	44	3555.0117	3555.01094	0.0008
349	1	40	3	37	0	41	3	38	3555.0337	3555.03376	-0.0001
350	1	40	3	38	0	41	3	39	3555.0348	3555.03444	0.0004
351	1	43	0	43	0	44	0	44	3555.0362	3555.03522	0.001
352	1	35	5	30	0	36	5	31	3555.0445	3555.04483	-0.0003
353	1	42	1	41	0	43	1	42	3555.0964	3555.09682	-0.0004
354	1	41	2	39	0	42	2	40	3555.1241	3555.12479	-0.0007
355	1	41	2	40	0	42	2	41	3555.1376	3555.13826	-0.0007
356	1	37	4	33	0	38	4	34	3555.1711	3555.17177	-0.0007
357	1	42	1	42	0	43	1	43	3555.1741	3555.17353	0.0006
358	1	31	6	25	0	32	6	26	3555.1859	3555.18539	0.0005
359	1	42	0	42	0	43	0	43	3555.1966	3555.19766	-0.0011
360	1	39	3	36	0	40	3	37	3555.2018	3555.20086	0.0009
361	1	39	3	37	0	40	3	38	3555.2026	3555.2016	0.001
362	1	34	5	29	0	35	5	30	3555.2221	3555.22189	0.0002
363	1	41	1	40	0	42	1	41	3555.2586	3555.25958	-0.001
364	1	40	2	39	0	41	2	40	3555.3041	3555.30367	0.0004
365	1	41	1	41	0	42	1	42	3555.3385	3555.33794	0.0006
366	1	36	4	32	0	37	4	33	3555.3452	3555.34486	0.0003
367	1	41	0	41	0	42	0	42	3555.3613	3555.36187	-0.0006
368	1	38	3	35	0	39	3	36	3555.3697	3555.36995	-0.0003
369	1	38	3	36	0	39	3	37	3555.3711	3555.37073	0.0004
370	1	33	5	28	0	34	5	29	3555.4014	3555.40089	0.0005
371	1	40	1	39	0	41	1	40	3555.424	3555.4243	-0.0003
372	1	40	1	40	0	41	1	41	3555.5036	3555.50418	-0.0006
373	1	35	4	31	0	36	4	32	3555.5197	3555.51993	-0.0002
374	1	40	0	40	0	41	0	41	3555.5286	3555.52788	0.0007
375	1	37	3	34	0	38	3	35	3555.5418	3555.54103	0.0008
376	1	37	3	35	0	38	3	36	3555.5419	3555.54183	0.0001
377	1	39	1	38	0	40	1	39	3555.5912	3555.59098	0.0002
378	1	39	1	39	0	40	1	40	3555.6715	3555.67224	-0.0007



379	1	39	0	39	0	40	0	40	3555.695	3555.69567	-0.0007
380	1	36	3	33	0	37	3	34	3555.7136	3555.7141	-0.0005
381	1	36	3	34	0	37	3	35	3555.7142	3555.71489	-0.0007
382	1	38	1	37	0	39	1	38	3555.7593	3555.75963	-0.0003
383	1	38	1	38	0	39	1	39	3555.8417	3555.84214	-0.0004
384	1	38	0	38	0	39	0	39	3555.8648	3555.86526	-0.0005
385	1	35	3	32	0	36	3	33	3555.8888	3555.88914	-0.0003
386	1	35	3	33	0	36	3	34	3555.8902	3555.88992	0.0003
387	1	37	1	36	0	38	1	37	3555.9306	3555.93026	0.0003
388	1	37	1	37	0	38	1	38	3556.013	3556.01386	-0.0009
389	1	37	0	37	0	38	0	38	3556.0358	3556.03665	-0.0008
390	1	34	3	31	0	35	3	32	3556.0662	3556.06616	0
391	1	34	3	32	0	35	3	33	3556.067	3556.06691	0.0001
392	1	36	1	35	0	37	1	36	3556.1031	3556.10288	0.0002
393	1	36	1	36	0	37	1	37	3556.1869	3556.18741	-0.0005
394	1	33	3	31	0	34	3	32	3556.2468	3556.24586	0.0009
395	1	10	10	0	0	10	10	1	3558.8341	3558.83462	-0.0005
396	1	10	10	0	0	10	10	1	3558.8355	3558.83462	0.0009
397	1	11	10	2	0	11	10	1	3558.8553	3558.85554	-0.0002
398	1	11	10	1	0	11	10	2	3558.8561	3558.85554	0.0006
399	1	12	10	2	0	12	10	3	3558.878	3558.87836	-0.0004
400	1	12	10	2	0	12	10	3	3558.8784	3558.87836	0
401	1	13	10	3	0	13	10	4	3558.9032	3558.90308	0.0001
402	1	13	10	3	0	13	10	4	3558.9041	3558.90308	0.001
403	1	14	10	4	0	14	10	5	3558.9289	3558.92969	-0.0008
404	1	14	10	4	0	14	10	5	3558.9303	3558.92969	0.0006
405	1	15	10	5	0	15	10	6	3558.9577	3558.95821	-0.0005
406	1	15	10	5	0	15	10	6	3558.9588	3558.95821	0.0006
407	1	9	9	0	0	9	9	1	3559.8007	3559.79968	0.001
408	1	10	9	1	0	10	9	2	3559.8182	3559.8187	-0.0005
409	1	11	9	2	0	11	9	3	3559.8391	3559.83962	-0.0005
410	1	12	9	3	0	12	9	4	3559.8616	3559.86244	-0.0008
411	1	13	9	4	0	13	9	5	3559.8861	3559.88716	-0.0011
412	1	14	9	5	0	14	9	6	3559.9144	3559.91378	0.0006
413	1	15	9	6	0	15	9	7	3559.9421	3559.94229	-0.0002
414	1	16	9	7	0	16	9	8	3559.9733	3559.97271	0.0006
415	1	8	8	0	0	8	8	1	3560.6678	3560.66702	0.0008
416	1	9	8	1	0	9	8	2	3560.6846	3560.68414	0.0005
417	1	10	8	2	0	10	8	3	3560.7033	3560.70316	0.0001
418	1	11	8	3	0	11	8	4	3560.7246	3560.72408	0.0005
419	1	12	8	4	0	12	8	5	3560.7465	3560.7469	-0.0004
420	1	13	8	5	0	13	8	6	3560.7713	3560.77162	-0.0003
421	1	14	8	6	0	14	8	7	3560.7977	3560.79824	-0.0005
422	1	15	8	7	0	15	8	8	3560.8268	3560.82676	0
423	1	7	7	0	0	7	7	1	3561.4349	3561.43532	-0.0004

424	1	8	7	1	0	8	7	2	3561.4514	3561.45053	0.0009
425	1	9	7	2	0	9	7	3	3561.4675	3561.46765	-0.0002
426	1	10	7	3	0	10	7	4	3561.486	3561.48668	-0.0007
427	1	11	7	4	0	11	7	5	3561.507	3561.5076	-0.0006
428	1	12	7	5	0	12	7	6	3561.5298	3561.53042	-0.0006
429	1	6	6	0	0	6	6	1	3562.1042	3562.10341	0.0008
430	1	7	6	1	0	7	6	2	3562.1173	3562.11672	0.0006
431	1	8	6	2	0	8	6	3	3562.1324	3562.13194	0.0005
432	1	9	6	3	0	9	6	4	3562.1487	3562.14906	-0.0004
433	1	10	6	4	0	10	6	5	3562.1673	3562.16808	-0.0008
434	1	11	6	5	0	11	6	6	3562.1885	3562.18901	-0.0005
435	1	12	6	6	0	12	6	7	3562.2113	3562.21183	-0.0005
436	1	13	6	7	0	13	6	8	3562.2357	3562.23655	-0.0009
437	1	5	5	0	0	5	5	1	3562.6702	3562.67028	-0.0001
438	1	6	5	1	0	6	5	2	3562.6818	3562.68169	0.0001
439	1	7	5	2	0	7	5	3	3562.6952	3562.69501	0.0002
440	1	8	5	3	0	8	5	4	3562.71	3562.71023	-0.0002
441	1	9	5	4	0	9	5	5	3562.727	3562.72735	-0.0004
442	1	10	5	5	0	10	5	6	3562.7457	3562.74637	-0.0007
443	1	11	5	6	0	11	5	7	3562.7672	3562.7673	-0.0001
444	1	4	4	0	0	4	4	1	3563.1359	3563.13507	0.0008
445	1	5	4	1	0	5	4	2	3563.1454	3563.14459	0.0008
446	1	6	4	2	0	6	4	3	3563.1567	3563.156	0.0007
447	1	7	4	3	0	7	4	4	3563.1696	3563.16932	0.0003
448	1	8	4	4	0	8	4	5	3563.185	3563.18454	0.0005
449	1	9	4	5	0	9	4	6	3563.2023	3563.20167	0.0006
450	1	10	4	6	0	10	4	7	3563.2211	3563.22069	0.0004
451	1	11	4	7	0	11	4	6	3565.9321	3565.93255	-0.0004
452	1	12	4	8	0	12	4	7	3566.2007	3566.19993	0.0008
453	1	13	4	9	0	13	4	8	3566.4697	3566.46919	0.0005
454	1	14	4	10	0	14	4	9	3566.7395	3566.74033	-0.0008
455	1	13	3	10	0	13	3	9	3566.8396	3566.83872	0.0009
456	1	15	4	11	0	15	4	10	3567.0138	3567.01335	0.0005
457	1	14	3	11	0	14	3	10	3567.11	3567.1099	0.0001
458	1	16	4	12	0	16	4	11	3567.289	3567.28824	0.0008
459	1	18	5	13	0	18	5	12	3567.3699	3567.36967	0.0002
460	1	15	3	12	0	15	3	11	3567.3828	3567.38297	-0.0002
461	1	17	4	13	0	17	4	12	3567.5644	3567.56501	-0.0006
462	1	19	5	14	0	19	5	13	3567.651	3567.65015	0.0008
463	1	16	3	13	0	16	3	12	3567.6572	3567.65793	-0.0007
464	1	15	1	15	0	15	1	14	3567.754	3567.75318	0.0008
465	1	18	4	14	0	18	4	13	3567.8445	3567.84365	0.0009
466	1	15	0	15	0	15	0	14	3567.8522	3567.85182	0.0004
467	1	15	1	14	0	15	1	13	3567.8529	3567.85368	-0.0008
468	1	16	2	15	0	16	2	14	3567.9198	3567.91985	0

469	1	20	5	15	0	19	5	14	3567.932	3567.9325	-0.0005
470	1	17	3	14	0	16	3	13	3567.9337	3567.93479	-0.0011
471	1	16	1	16	0	15	1	15	3568.0227	3568.02358	-0.0009
472	1	19	4	15	0	18	4	14	3568.1234	3568.12416	-0.0008
473	1	16	0	16	0	15	0	15	3568.1252	3568.12516	0
474	1	16	1	15	0	15	1	14	3568.1327	3568.13207	0.0006
475	1	17	2	16	0	16	2	15	3568.1968	3568.19619	0.0006
476	1	18	3	15	0	17	3	14	3568.2144	3568.21353	0.0009
477	1	21	5	16	0	20	5	15	3568.2161	3568.21671	-0.0006
478	1	17	1	17	0	16	1	16	3568.2963	3568.2957	0.0006
479	1	17	0	17	0	16	0	16	3568.3996	3568.40016	-0.0006
480	1	20	4	16	0	19	4	15	3568.4061	3568.40653	-0.0004
481	1	17	1	16	0	16	1	15	3568.4119	3568.41235	-0.0004
482	1	18	2	17	0	17	2	16	3568.4739	3568.47436	-0.0005
483	1	19	3	16	0	18	3	15	3568.4938	3568.49416	-0.0004
484	1	22	5	17	0	21	5	16	3568.5035	3568.50278	0.0007
485	1	18	1	18	0	17	1	17	3568.5691	3568.56954	-0.0004
486	1	18	0	18	0	17	0	17	3568.6768	3568.67678	0
487	1	21	4	17	0	20	4	16	3568.6915	3568.69077	0.0007
488	1	18	1	17	0	17	1	16	3568.6943	3568.69449	-0.0002
489	1	19	2	18	0	18	2	17	3568.7547	3568.75433	0.0004
490	1	20	3	17	0	19	3	16	3568.7767	3568.77669	0
491	1	23	5	18	0	22	5	17	3568.79	3568.7907	-0.0007
492	1	19	1	19	0	18	1	18	3568.8446	3568.8451	-0.0005
493	1	19	0	19	0	18	0	18	3568.9547	3568.95501	-0.0003
494	1	22	4	18	0	21	4	17	3568.9763	3568.97688	-0.0006
495	1	19	1	18	0	18	1	17	3568.9787	3568.9785	0.0002
496	1	20	2	19	0	19	2	18	3569.0356	3569.03611	-0.0005
497	1	21	3	18	0	20	3	17	3569.0602	3569.0611	-0.0009
498	1	24	5	19	0	23	5	18	3569.0811	3569.08047	0.0006
499	1	31	8	23	0	30	8	22	3569.1206	3569.11993	0.0007
500	1	20	1	20	0	19	1	19	3569.122	3569.12236	-0.0004
501	1	20	0	20	0	19	0	19	3569.2341	3569.23483	-0.0007
502	1	23	4	19	0	22	4	18	3569.2641	3569.26485	-0.0007
503	1	20	1	19	0	19	1	18	3569.2651	3569.26437	0.0007
504	1	21	2	20	0	20	2	19	3569.3198	3569.31968	0.0001
505	1	22	3	19	0	21	3	18	3569.3467	3569.34741	-0.0007
506	1	25	5	20	0	24	5	19	3569.3721	3569.37208	0
507	1	21	1	21	0	20	1	20	3569.4005	3569.40133	-0.0008
508	1	32	8	24	0	31	8	23	3569.4238	3569.42436	-0.0006
509	1	21	0	21	0	20	0	20	3569.5165	3569.51621	0.0003
510	1	21	1	20	0	20	1	19	3569.5531	3569.55208	0.001
511	1	24	4	20	0	23	4	19	3569.555	3569.55468	0.0003
512	1	22	2	21	0	21	2	20	3569.6052	3569.60505	0.0002
513	1	23	3	20	0	22	3	19	3569.6362	3569.63561	0.0006

514	1	26	5	21	0	25	5	20	3569.6651	3569.66555	-0.0004
515	1	22	1	22	0	21	1	21	3569.6811	3569.68198	-0.0009
516	1	33	8	25	0	32	8	24	3569.7308	3569.73061	0.0002
517	1	22	0	22	0	21	0	21	3569.7982	3569.79914	-0.0009
518	1	22	1	21	0	21	1	20	3569.8407	3569.84162	-0.0009
519	1	25	4	21	0	24	4	20	3569.8458	3569.84637	-0.0006
520	1	23	2	22	0	22	2	21	3569.8921	3569.89219	-0.0001
521	1	31	7	24	0	30	7	23	3569.9021	3569.90211	0
522	1	23	2	21	0	22	2	20	3569.9166	3569.91616	0.0004
523	1	24	3	21	0	23	3	20	3569.9259	3569.92571	0.0002
524	1	27	5	22	0	26	5	21	3569.9614	3569.96085	0.0005
525	1	23	1	23	0	22	1	22	3569.9648	3569.96433	0.0005
526	1	34	8	26	0	33	8	25	3570.0378	3570.03866	-0.0009
527	1	23	0	23	0	22	0	22	3570.0837	3570.0836	0.0001
528	1	23	1	22	0	22	1	21	3570.1339	3570.13299	0.0009
529	1	26	4	22	0	25	4	21	3570.1406	3570.13991	0.0007
530	1	24	2	23	0	23	2	22	3570.1807	3570.18112	-0.0004
531	1	32	7	25	0	31	7	24	3570.2058	3570.20652	-0.0007
532	1	24	2	22	0	23	2	21	3570.2089	3570.20863	0.0003
533	1	25	3	22	0	24	3	21	3570.2178	3570.2177	0.0001
534	1	24	1	24	0	23	1	23	3570.2474	3570.24835	-0.0009
535	1	28	5	23	0	27	5	22	3570.2588	3570.258	0.0008
536	1	35	8	27	0	34	8	26	3570.3489	3570.34851	0.0004
537	1	24	0	24	0	23	0	23	3570.3705	3570.36956	0.0009
538	1	24	1	23	0	23	1	22	3570.4258	3570.42616	-0.0004
539	1	27	4	23	0	26	4	22	3570.4349	3570.43531	-0.0004
540	1	25	2	24	0	24	2	23	3570.4718	3570.47181	0
541	1	25	2	23	0	24	2	22	3570.5023	3570.50321	-0.0009
542	1	26	3	23	0	25	3	22	3570.5115	3570.5116	-0.0001
543	1	33	7	26	0	32	7	25	3570.5136	3570.51275	0.0008
544	1	25	1	25	0	24	1	24	3570.5345	3570.53404	0.0005
545	1	29	5	24	0	28	5	23	3570.5574	3570.55699	0.0004
546	1	25	0	25	0	24	0	24	3570.6564	3570.65702	-0.0006
547	1	36	8	28	0	35	8	27	3570.661	3570.66017	0.0008
548	1	25	1	24	0	24	1	23	3570.7204	3570.72114	-0.0007
549	1	28	4	24	0	27	4	23	3570.7319	3570.73256	-0.0007
550	1	26	2	25	0	25	2	24	3570.7644	3570.76427	0.0001
551	1	26	2	24	0	25	2	23	3570.7991	3570.79991	-0.0008
552	1	27	3	24	0	26	3	23	3570.8069	3570.80739	-0.0005
553	1	34	7	27	0	33	7	26	3570.8202	3570.82079	-0.0006
554	1	26	1	26	0	25	1	25	3570.8222	3570.8214	0.0008
555	1	30	5	25	0	29	5	24	3570.8578	3570.85781	0
556	1	32	6	26	0	31	6	25	3570.8861	3570.88699	-0.0009
557	1	26	0	26	0	25	0	25	3570.9467	3570.94594	0.0008
558	1	37	8	29	0	36	8	28	3570.9727	3570.97362	-0.0009

559	1	26	1	25	0	25	1	24	3571.0173	3571.0179	-0.0006
560	1	29	4	25	0	28	4	24	3571.0324	3571.03166	0.0007
561	1	27	2	26	0	26	2	25	3571.0594	3571.05847	0.0009
562	1	27	2	25	0	26	2	24	3571.0991	3571.09874	0.0004
563	1	28	3	25	0	27	3	24	3571.1047	3571.10508	-0.0004
564	1	27	1	27	0	26	1	26	3571.1112	3571.11042	0.0008
565	1	35	7	28	0	34	7	27	3571.1314	3571.13064	0.0008
566	1	31	5	26	0	30	5	25	3571.1602	3571.16046	-0.0003
567	1	33	6	27	0	32	6	26	3571.1924	3571.19323	-0.0008
568	1	27	0	27	0	26	0	26	3571.2357	3571.23632	-0.0006
569	1	38	8	30	0	37	8	29	3571.2888	3571.28887	-0.0001
570	1	27	1	26	0	26	1	25	3571.3169	3571.31644	0.0005
571	1	30	4	26	0	29	4	25	3571.3333	3571.33261	0.0007
572	1	28	2	27	0	27	2	26	3571.3541	3571.35443	-0.0003
573	1	28	2	26	0	27	2	25	3571.399	3571.39969	-0.0007
574	1	28	1	28	0	27	1	27	3571.4004	3571.40109	-0.0007
575	1	29	3	26	0	28	3	25	3571.4051	3571.40468	0.0004
576	1	36	7	29	0	35	7	28	3571.4418	3571.44229	-0.0005
577	1	32	5	27	0	31	5	26	3571.4641	3571.46494	-0.0008
578	1	34	6	28	0	33	6	27	3571.501	3571.50129	-0.0003
579	1	28	0	28	0	27	0	27	3571.5275	3571.52814	-0.0006
580	1	39	8	31	0	38	8	30	3571.6062	3571.60591	0.0003
581	1	28	1	27	0	27	1	26	3571.6173	3571.61674	0.0006
582	1	31	4	27	0	30	4	26	3571.6358	3571.63541	0.0004
583	1	29	2	28	0	28	2	27	3571.6531	3571.65212	0.001
584	1	29	1	29	0	28	1	28	3571.6937	3571.6934	0.0003
585	1	29	2	27	0	28	2	26	3571.703	3571.70277	0.0002
586	1	30	3	27	0	29	3	26	3571.706	3571.70619	-0.0002
587	1	37	7	30	0	36	7	29	3571.7563	3571.75575	0.0006
588	1	33	5	28	0	32	5	27	3571.7704	3571.77125	-0.0008
589	1	35	6	29	0	34	6	28	3571.8109	3571.81116	-0.0003
590	1	29	0	29	0	28	0	28	3571.8207	3571.82138	-0.0007
591	1	29	1	28	0	28	1	27	3571.9184	3571.91879	-0.0004
592	1	40	8	32	0	39	8	31	3571.9243	3571.92473	-0.0004
593	1	32	4	28	0	31	4	27	3571.9406	3571.94005	0.0005
594	1	30	2	29	0	29	2	28	3571.9516	3571.95154	0.0001
595	1	30	1	30	0	29	1	29	3571.9882	3571.98735	0.0008
596	1	30	2	28	0	29	2	27	3572.0084	3572.00799	0.0004
597	1	31	3	28	0	30	3	27	3572.0098	3572.00961	0.0002
598	1	38	7	31	0	37	7	30	3572.0704	3572.071	-0.0006
599	1	34	5	29	0	33	5	28	3572.0791	3572.07938	-0.0003
600	1	30	0	30	0	29	0	29	3572.1152	3572.11604	-0.0008
601	1	36	6	30	0	35	6	29	3572.1236	3572.12284	0.0008
602	1	30	1	29	0	29	1	28	3572.2225	3572.22257	-0.0001
603	1	41	8	33	0	40	8	32	3572.2447	3572.24533	-0.0006

604	1	33	4	29	0	32	4	28	3572.2473	3572.24654	0.0008
605	1	31	2	30	0	30	2	29	3572.252	3572.25269	-0.0007
606	1	31	1	31	0	30	1	30	3572.2824	3572.28294	-0.0005
607	1	32	3	29	0	31	3	28	3572.3147	3572.31495	-0.0002
608	1	31	2	29	0	30	2	28	3572.3155	3572.31533	0.0002
609	1	39	7	32	0	38	7	31	3572.3877	3572.38804	-0.0003
610	1	35	5	30	0	34	5	29	3572.3892	3572.38934	-0.0001
611	1	31	0	31	0	30	0	30	3572.4121	3572.41209	0
612	1	37	6	31	0	36	6	30	3572.4369	3572.43633	0.0006
613	1	31	1	30	0	30	1	29	3572.5282	3572.52808	0.0001
614	1	34	4	30	0	33	4	29	3572.5544	3572.55487	-0.0005
615	1	32	2	31	0	31	2	30	3572.5558	3572.55555	0.0003
616	1	42	8	34	0	41	8	33	3572.5683	3572.56772	0.0006
617	1	32	1	32	0	31	1	31	3572.5811	3572.58014	0.001
618	1	33	3	30	0	32	3	29	3572.6222	3572.6222	0
619	1	32	2	30	0	31	2	29	3572.6257	3572.6248	0.0009
620	1	36	5	31	0	35	5	30	3572.7021	3572.70111	0.001
621	1	40	7	33	0	39	7	32	3572.7069	3572.70687	0
622	1	32	0	32	0	31	0	31	3572.7099	3572.70953	0.0004
623	1	32	1	31	0	31	1	30	3572.8353	3572.83529	0
624	1	33	2	32	0	32	2	31	3572.8607	3572.86011	0.0006
625	1	35	4	31	0	34	4	30	3572.8642	3572.86503	-0.0008
626	1	33	1	33	0	32	1	32	3572.8788	3572.87896	-0.0002
627	1	43	8	35	0	42	8	34	3572.8929	3572.89187	0.001
628	1	34	3	32	0	33	3	31	3572.9264	3572.92639	0
629	1	34	3	31	0	33	3	30	3572.9305	3572.93137	-0.0009
630	1	33	2	31	0	32	2	30	3572.9357	3572.9364	-0.0007
631	1	33	0	33	0	32	0	32	3573.0088	3573.00835	0.0004
632	1	37	5	32	0	36	5	31	3573.0155	3573.01469	0.0008
633	1	41	7	34	0	40	7	33	3573.0273	3573.02749	-0.0002
634	1	33	1	32	0	32	1	31	3573.1445	3573.14418	0.0003
635	1	34	2	33	0	33	2	32	3573.1663	3573.16638	-0.0001
636	1	36	4	32	0	35	4	31	3573.1761	3573.17704	-0.0009
637	1	34	1	34	0	33	1	33	3573.1798	3573.1794	0.0004
638	1	44	8	36	0	43	8	35	3573.2179	3573.2178	0.0001
639	1	35	3	33	0	34	3	32	3573.2363	3573.23666	-0.0004
640	1	35	3	32	0	34	3	31	3573.2432	3573.24248	0.0007
641	1	34	2	32	0	33	2	31	3573.2495	3573.25011	-0.0006
642	1	34	0	34	0	33	0	33	3573.3094	3573.30855	0.0009
643	1	38	5	33	0	37	5	32	3573.3307	3573.33009	0.0006
644	1	42	7	35	0	41	7	34	3573.3495	3573.34989	-0.0004
645	1	34	1	33	0	33	1	32	3573.4539	3573.45475	-0.0009
646	1	35	2	34	0	34	2	33	3573.4749	3573.47433	0.0006
647	1	35	1	35	0	34	1	34	3573.482	3573.48143	0.0006
648	1	37	4	33	0	36	4	32	3573.4905	3573.49088	-0.0004

649	1	45	8	37	0	44	8	36	3573.5458	3573.54549	0.0003
650	1	36	3	34	0	35	3	33	3573.549	3573.54875	0.0003
651	1	36	3	33	0	35	3	32	3573.5559	3573.55551	0.0004
652	1	35	2	33	0	34	2	32	3573.5658	3573.56594	-0.0001
653	1	35	0	35	0	34	0	34	3573.6091	3573.61011	-0.001
654	1	39	5	34	0	38	5	33	3573.6466	3573.6473	-0.0007
655	1	43	7	36	0	42	7	35	3573.6741	3573.67407	0
656	1	35	1	34	0	34	1	33	3573.7677	3573.76698	0.0007
657	1	36	2	35	0	35	2	34	3573.7838	3573.78396	-0.0002
658	1	36	1	36	0	35	1	35	3573.7849	3573.78507	-0.0002
659	1	38	4	34	0	37	4	33	3573.8061	3573.80656	-0.0005
660	1	37	3	35	0	36	3	34	3573.8636	3573.86266	0.0009
661	1	37	3	34	0	36	3	33	3573.8711	3573.87049	0.0006
662	1	46	8	38	0	45	8	37	3573.8747	3573.87495	-0.0002
663	1	36	2	34	0	35	2	33	3573.8843	3573.88386	0.0004
664	1	36	0	36	0	35	0	35	3573.9134	3573.91305	0.0004
665	1	40	5	35	0	39	5	34	3573.9662	3573.96632	-0.0001
666	1	44	7	37	0	43	7	36	3574.0004	3574.00002	0.0004
667	1	36	1	35	0	35	1	34	3574.0806	3574.08085	-0.0002
668	1	37	1	37	0	36	1	36	3574.0912	3574.09029	0.0009
669	1	37	2	36	0	36	2	35	3574.0958	3574.09526	0.0005
670	1	39	4	35	0	38	4	34	3574.1235	3574.12407	-0.0006
671	1	38	3	36	0	37	3	35	3574.1794	3574.17837	0.001
672	1	38	3	35	0	37	3	34	3574.1868	3574.1874	-0.0006
673	1	37	2	35	0	36	2	34	3574.2029	3574.20387	-0.001
674	1	47	8	39	0	46	8	38	3574.2069	3574.20616	0.0007
675	1	37	0	37	0	36	0	36	3574.2178	3574.21734	0.0005
676	1	41	5	36	0	40	5	35	3574.2867	3574.28714	-0.0004
677	1	45	7	38	0	44	7	37	3574.3286	3574.32775	0.0009
678	1	38	1	38	0	37	1	37	3574.397	3574.39711	-0.0001
679	1	37	1	36	0	36	1	35	3574.397	3574.39633	0.0007
680	1	38	2	37	0	37	2	36	3574.4087	3574.40823	0.0005
681	1	40	4	36	0	39	4	35	3574.4437	3574.44341	0.0003
682	1	39	3	37	0	38	3	36	3574.4953	3574.4959	-0.0006
683	1	39	3	36	0	38	3	35	3574.5058	3574.50627	-0.0005
684	1	38	0	38	0	37	0	37	3574.5233	3574.523	0.0003
685	1	38	2	36	0	37	2	35	3574.5258	3574.52595	-0.0001
686	1	42	5	37	0	41	5	36	3574.6095	3574.60976	-0.0003
687	1	46	7	39	0	45	7	38	3574.6567	3574.65724	-0.0005
688	1	39	1	39	0	38	1	38	3574.7056	3574.7055	0.0001
689	1	38	1	37	0	37	1	36	3574.7144	3574.71343	0.001
690	1	39	2	38	0	38	2	37	3574.7222	3574.72285	-0.0006
691	1	41	4	37	0	40	4	36	3574.7653	3574.76458	0.0007
692	1	40	3	38	0	39	3	37	3574.816	3574.81522	0.0008
693	1	40	3	37	0	39	3	36	3574.8281	3574.82709	0.001

694	1	39	0	39	0	38	0	38	3574.8297	3574.83003	-0.0003
695	1	39	2	37	0	38	2	36	3574.8508	3574.85008	0.0007
696	1	43	5	38	0	42	5	37	3574.9344	3574.93418	0.0002
697	1	47	7	40	0	46	7	39	3574.9882	3574.98849	-0.0003
698	1	40	1	40	0	39	1	39	3575.016	3575.01546	0.0005
699	1	39	1	38	0	38	1	37	3575.0318	3575.0321	-0.0003
700	1	40	2	39	0	39	2	38	3575.0399	3575.03912	0.0008
701	1	42	4	38	0	41	4	37	3575.0869	3575.08757	-0.0007
702	1	41	3	39	0	40	3	38	3575.136	3575.13633	-0.0003
703	1	40	0	40	0	39	0	39	3575.139	3575.13843	0.0006
704	1	41	3	38	0	40	3	37	3575.1505	3575.14988	0.0006
705	1	40	2	38	0	39	2	37	3575.1769	3575.17626	0.0006
706	1	41	1	41	0	40	1	40	3575.327	3575.327	0
707	1	40	1	39	0	39	1	38	3575.3525	3575.35235	0.0002
708	1	41	2	40	0	40	2	39	3575.3568	3575.35702	-0.0002
709	1	43	4	39	0	42	4	38	3575.4125	3575.4124	0.0001
710	1	41	0	41	0	40	0	40	3575.4488	3575.4482	0.0006
711	1	42	3	40	0	41	3	39	3575.4585	3575.45923	-0.0007
712	1	42	3	39	0	41	3	38	3575.4743	3575.47463	-0.0003
713	1	41	2	39	0	40	2	38	3575.5054	3575.50445	0.0009
714	1	42	1	42	0	41	1	41	3575.6396	3575.64009	-0.0005
715	1	41	1	40	0	40	1	39	3575.6736	3575.67414	-0.0005
716	1	42	2	41	0	41	2	40	3575.677	3575.67654	0.0005
717	1	44	4	40	0	43	4	39	3575.7399	3575.73905	0.0008
718	1	42	0	42	0	41	0	41	3575.7591	3575.75935	-0.0003
719	1	43	3	41	0	42	3	40	3575.7835	3575.78391	-0.0004
720	1	43	3	40	0	42	3	39	3575.8005	3575.80136	-0.0009
721	1	42	2	40	0	41	2	39	3575.8355	3575.83464	0.0009
722	1	43	1	43	0	42	1	42	3575.9553	3575.95474	0.0006
723	1	42	1	41	0	41	1	40	3575.9973	3575.99745	-0.0002
724	1	43	2	42	0	42	2	41	3575.9981	3575.99769	0.0004
725	1	45	4	41	0	44	4	40	3576.0676	3576.06753	0.0001
726	1	43	0	43	0	42	0	42	3576.0715	3576.07189	-0.0004
727	1	44	3	42	0	43	3	41	3576.1113	3576.11035	0.0009
728	1	44	3	41	0	43	3	40	3576.1291	3576.13007	-0.001
729	1	43	2	41	0	42	2	40	3576.1661	3576.16681	-0.0007
730	1	44	1	44	0	43	1	43	3576.2711	3576.27094	0.0002
731	1	44	2	43	0	43	2	42	3576.3196	3576.32045	-0.0008
732	1	43	1	42	0	42	1	41	3576.3217	3576.32228	-0.0006
733	1	44	0	44	0	43	0	43	3576.3866	3576.38583	0.0008
734	1	46	4	42	0	45	4	41	3576.3974	3576.39783	-0.0004
735	1	45	3	43	0	44	3	42	3576.4387	3576.43857	0.0001
736	1	45	3	42	0	44	3	41	3576.4618	3576.46077	0.001
737	1	44	2	42	0	43	2	41	3576.5014	3576.50093	0.0005
738	1	45	1	45	0	44	1	44	3576.588	3576.58869	-0.0007



739	1	45	2	44	0	44	2	43	3576.6442	3576.6448	-0.0006
740	1	44	1	43	0	43	1	42	3576.6496	3576.64858	0.001
741	1	45	0	45	0	44	0	44	3576.7009	3576.70118	-0.0003
742	1	47	4	43	0	46	4	42	3576.7303	3576.72995	0.0004
743	1	46	3	44	0	45	3	43	3576.7677	3576.76853	-0.0008
744	1	46	3	43	0	45	3	42	3576.7942	3576.79348	0.0007
745	1	45	2	43	0	44	2	42	3576.8363	3576.83697	-0.0007
746	1	46	1	46	0	45	1	45	3576.9074	3576.90798	-0.0006
747	1	46	2	45	0	45	2	44	3576.9704	3576.97075	-0.0003
748	1	45	1	44	0	44	1	43	3576.9767	3576.97636	0.0003
749	1	46	0	46	0	45	0	45	3577.0189	3577.01794	0.001
750	1	48	4	44	0	47	4	43	3577.0633	3577.06389	-0.0006
751	1	47	3	45	0	46	3	44	3577.1009	3577.10025	0.0007
752	1	47	3	44	0	46	3	43	3577.1273	3577.12818	-0.0009
753	1	46	2	44	0	45	2	43	3577.1742	3577.17492	-0.0007
754	1	47	1	47	0	46	1	46	3577.2283	3577.22881	-0.0005
755	1	47	2	46	0	46	2	45	3577.2991	3577.29827	0.0008
756	1	46	1	45	0	45	1	44	3577.3063	3577.30557	0.0007
757	1	47	0	47	0	46	0	46	3577.3357	3577.33612	-0.0004
758	1	52	6	46	0	51	6	45	3577.3537	3577.353	0.0007
759	1	49	4	45	0	48	4	44	3577.4	3577.39966	0.0003
760	1	48	3	46	0	47	3	45	3577.4329	3577.4337	-0.0008
761	1	48	3	45	0	47	3	44	3577.4653	3577.46491	0.0004
762	1	47	2	45	0	46	2	44	3577.5155	3577.51474	0.0008
763	1	47	1	46	0	46	1	45	3577.6355	3577.6362	-0.0007
764	1	48	0	48	0	47	0	47	3577.6561	3577.65574	0.0004
765	1	53	6	47	0	52	6	46	3577.6958	3577.6949	0.0009
766	1	50	4	46	0	49	4	45	3577.7372	3577.73724	0
767	1	49	3	47	0	48	3	46	3577.7697	3577.76889	0.0008
768	1	49	3	46	0	48	3	45	3577.8036	3577.80365	-0.0001
769	1	48	1	47	0	47	1	46	3577.9677	3577.96823	-0.0005
770	1	54	6	48	0	53	6	47	3578.0384	3578.03854	-0.0001
771	1	51	4	48	0	50	4	47	3578.0738	3578.07447	-0.0007
772	1	51	4	47	0	50	4	46	3578.0775	3578.07665	0.0009
773	1	50	3	48	0	49	3	47	3578.1048	3578.10579	-0.001
774	1	50	3	47	0	49	3	46	3578.1452	3578.14443	0.0008
775	1	55	6	49	0	54	6	48	3578.3844	3578.38393	0.0005
776	1	52	4	49	0	51	4	48	3578.4145	3578.41536	-0.0009
777	1	52	4	48	0	51	4	47	3578.4182	3578.41787	0.0003
778	1	51	3	49	0	50	3	48	3578.4445	3578.44441	0.0001
779	1	51	3	48	0	50	3	47	3578.488	3578.48725	0.0008
780	1	56	6	50	0	55	6	49	3578.7305	3578.73104	-0.0005
781	1	53	4	50	0	52	4	49	3578.7587	3578.75802	0.0007
782	1	53	4	49	0	52	4	48	3578.7618	3578.76091	0.0009
783	1	52	3	50	0	51	3	49	3578.7844	3578.78473	-0.0003

784	1	52	3	49	0	51	3	48	3578.8314	3578.83211	-0.0007
785	1	57	6	51	0	56	6	50	3579.0809	3579.0799	0.001
786	1	54	4	51	0	53	4	50	3579.1027	3579.10246	0.0002
787	1	54	4	50	0	53	4	49	3579.1052	3579.10578	-0.0006
788	1	53	3	51	0	52	3	50	3579.1266	3579.12674	-0.0001
789	1	53	3	50	0	52	3	49	3579.1784	3579.17902	-0.0006
790	1	58	6	52	0	57	6	51	3579.4307	3579.43047	0.0002
791	1	55	4	52	0	54	4	51	3579.4497	3579.44866	0.001
792	1	55	4	51	0	54	4	50	3579.4516	3579.45246	-0.0009
793	1	59	6	53	0	58	6	52	3579.7829	3579.78277	0.0001
794	1	56	4	53	0	55	4	52	3579.7972	3579.79663	0.0006
795	1	56	4	52	0	55	4	51	3579.8015	3579.80096	0.0005
796	1	57	4	54	0	56	4	53	3580.1468	3580.14635	0.0004
797	1	57	4	53	0	56	4	52	3580.1517	3580.15128	0.0004
798	1	58	4	55	0	57	4	54	3580.4973	3580.49783	-0.0005
799	1	58	4	54	0	57	4	53	3580.5038	3580.50343	0.0004
800	1	62	6	56	0	61	6	55	3580.8505	3580.84997	0.0005

B.3  $^{81}\text{BrNO } 2\nu_1$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu''$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	61	6	55	0	62	6	56	3550.6137	3550.61302	0.0007
2	1	58	6	52	0	59	6	53	3550.9936	3550.99409	-0.0005
3	1	57	6	51	0	58	6	52	3551.124	3551.12503	-0.001
4	1	56	6	50	0	57	6	51	3551.2576	3551.25791	-0.0003
5	1	45	8	37	0	46	8	38	3551.3792	3551.37879	0.0004
6	1	55	6	49	0	56	6	50	3551.392	3551.39275	-0.0008
7	1	54	6	48	0	55	6	49	3551.5291	3551.52955	-0.0004
8	1	44	8	36	0	45	8	37	3551.536	3551.53524	0.0008
9	1	53	6	47	0	54	6	48	3551.6677	3551.6683	-0.0006
10	1	43	8	35	0	44	8	36	3551.6927	3551.69363	-0.0009
11	1	52	6	46	0	53	6	47	3551.8099	3551.809	0.0009
12	1	42	8	34	0	43	8	35	3551.8541	3551.85398	0.0001
13	1	51	6	45	0	52	6	46	3551.951	3551.95166	-0.0007
14	1	41	8	33	0	42	8	34	3552.0172	3552.01627	0.0009
15	1	40	8	32	0	41	8	33	3552.1799	3552.18051	-0.0006
16	1	57	4	54	0	58	4	55	3552.183	3552.18351	-0.0005
17	1	57	4	53	0	58	4	54	3552.1834	3552.18428	-0.0009
18	1	56	4	53	0	57	4	54	3552.3153	3552.3161	-0.0008
19	1	56	4	52	0	57	4	53	3552.3174	3552.31674	0.0007
20	1	44	7	37	0	45	7	38	3552.3214	3552.32135	0
21	1	39	8	31	0	40	8	32	3552.3457	3552.3467	-0.001
22	1	55	4	52	0	56	4	53	3552.4504	3552.45066	-0.0003
23	1	55	4	51	0	56	4	52	3552.4505	3552.45118	-0.0007

24	1	43	7	36	0	44	7	37	3552.4803	3552.47969	0.0006
25	1	38	8	30	0	39	8	31	3552.5139	3552.51483	-0.0009
26	1	54	4	51	0	55	4	52	3552.5867	3552.58719	-0.0005
27	1	54	4	50	0	55	4	51	3552.5871	3552.58761	-0.0005
28	1	42	7	35	0	43	7	36	3552.6405	3552.63998	0.0005
29	1	37	8	29	0	38	8	30	3552.6856	3552.68491	0.0007
30	1	53	4	50	0	54	4	51	3552.7259	3552.72568	0.0002
31	1	53	4	49	0	54	4	50	3552.7271	3552.72603	0.0011
32	1	41	7	34	0	42	7	35	3552.802	3552.80221	-0.0002
33	1	36	8	28	0	37	8	29	3552.8571	3552.85693	0.0002
34	1	52	4	48	0	53	4	49	3552.8658	3552.86642	-0.0006
35	1	52	4	49	0	53	4	50	3552.8661	3552.86615	0
36	1	40	7	33	0	41	7	34	3552.9663	3552.9664	-0.0001
37	1	51	4	48	0	52	4	49	3553.0078	3553.00858	-0.0008
38	1	51	4	47	0	52	4	48	3553.0079	3553.0088	-0.0009
39	1	35	8	27	0	36	8	28	3553.0316	3553.0309	0.0007
40	1	39	7	32	0	40	7	33	3553.133	3553.13253	0.0005
41	1	50	4	46	0	51	4	47	3553.1535	3553.15315	0.0004
42	1	34	8	26	0	35	8	27	3553.2072	3553.20681	0.0004
43	1	49	4	45	0	50	4	46	3553.2994	3553.29947	-0.0001
44	1	38	7	31	0	39	7	32	3553.3	3553.30061	-0.0006
45	1	51	3	49	0	52	3	50	3553.3787	3553.3789	-0.0002
46	1	51	3	48	0	52	3	49	3553.3825	3553.38213	0.0004
47	1	33	8	25	0	34	8	26	3553.3855	3553.38466	0.0008
48	1	48	4	44	0	49	4	45	3553.4477	3553.44777	-0.0001
49	1	37	7	30	0	38	7	31	3553.4706	3553.47063	0
50	1	50	3	48	0	51	3	49	3553.5238	3553.52334	0.0005
51	1	50	3	47	0	51	3	48	3553.526	3553.52586	0.0001
52	1	32	8	24	0	33	8	25	3553.5643	3553.56446	-0.0002
53	1	47	4	43	0	48	4	44	3553.5982	3553.59804	0.0002
54	1	36	7	29	0	37	7	30	3553.642	3553.64261	-0.0006
55	1	49	3	47	0	50	3	48	3553.6697	3553.66973	0
56	1	49	3	46	0	50	3	47	3553.6723	3553.67163	0.0007
57	1	31	8	23	0	32	8	24	3553.7459	3553.7462	-0.0003
58	1	46	4	42	0	47	4	43	3553.7498	3553.75028	-0.0005
59	1	35	7	28	0	36	7	29	3553.8169	3553.81652	0.0004
60	1	48	3	46	0	49	3	47	3553.8179	3553.81807	-0.0002
61	1	48	3	45	0	49	3	46	3553.8192	3553.81945	-0.0002
62	1	42	5	37	0	43	5	38	3553.9032	3553.90342	-0.0002
63	1	45	4	41	0	46	4	42	3553.9047	3553.90449	0.0002
64	1	30	8	22	0	31	8	23	3553.9298	3553.92989	-0.0001
65	1	47	3	45	0	48	3	46	3553.968	3553.96837	-0.0004
66	1	47	3	44	0	48	3	45	3553.9689	3553.96929	-0.0004
67	1	34	7	27	0	35	7	28	3553.9922	3553.99239	-0.0002
68	1	34	7	27	0	35	7	28	3553.9931	3553.99239	0.0007

69	1	44	4	40	0	45	4	41	3554.0611	3554.06067	0.0004
70	1	41	5	36	0	42	5	37	3554.0652	3554.06555	-0.0004
71	1	46	3	44	0	47	3	45	3554.1207	3554.12062	0.0001
72	1	46	3	43	0	47	3	44	3554.1214	3554.12116	0.0002
73	1	33	7	26	0	34	7	27	3554.1691	3554.17019	-0.0011
74	1	43	4	39	0	44	4	40	3554.2197	3554.21881	0.0009
75	1	40	5	35	0	41	5	36	3554.2298	3554.22963	0.0002
76	1	45	3	42	0	46	3	43	3554.2754	3554.27505	0.0003
77	1	36	6	30	0	37	6	31	3554.3255	3554.3258	-0.0003
78	1	32	7	25	0	33	7	26	3554.3503	3554.34994	0.0004
79	1	42	4	38	0	43	4	39	3554.3797	3554.37891	0.0008
80	1	39	5	34	0	40	5	35	3554.3961	3554.39567	0.0004
81	1	44	3	41	0	45	3	42	3554.4311	3554.43095	0.0001
82	1	35	6	29	0	36	6	30	3554.4988	3554.49968	-0.0009
83	1	31	7	24	0	32	7	25	3554.5315	3554.53163	-0.0001
84	1	45	2	43	0	46	2	44	3554.5347	3554.53422	0.0005
85	1	41	4	37	0	42	4	38	3554.5413	3554.54097	0.0003
86	1	45	2	44	0	46	2	45	3554.5428	3554.54223	0.0006
87	1	38	5	33	0	39	5	34	3554.5636	3554.56365	-0.0001
88	1	46	1	46	0	47	1	47	3554.5798	3554.58061	-0.0008
89	1	43	3	40	0	44	3	41	3554.5885	3554.58886	-0.0004
90	1	43	3	41	0	44	3	42	3554.5885	3554.58911	-0.0006
91	1	45	1	44	0	46	1	45	3554.6686	3554.66763	0.001
92	1	34	6	28	0	35	6	29	3554.6755	3554.67549	0
93	1	44	2	42	0	45	2	43	3554.6887	3554.68937	-0.0007
94	1	44	2	43	0	45	2	44	3554.6985	3554.69884	-0.0003
95	1	40	4	36	0	41	4	37	3554.7059	3554.705	0.0009
96	1	30	7	23	0	31	7	24	3554.7158	3554.71527	0.0005
97	1	37	5	32	0	38	5	33	3554.7328	3554.73359	-0.0008
98	1	45	1	45	0	46	1	46	3554.7361	3554.7366	-0.0005
99	1	42	3	39	0	43	3	40	3554.7482	3554.74877	-0.0006
100	1	42	3	40	0	43	3	41	3554.7487	3554.74918	-0.0005
101	1	45	0	45	0	46	0	46	3554.7621	3554.76153	0.0006
102	1	44	1	43	0	45	1	44	3554.8231	3554.82339	-0.0003
103	1	43	2	41	0	44	2	42	3554.8472	3554.84659	0.0006
104	1	33	6	27	0	34	6	28	3554.8522	3554.85326	-0.0011
105	1	43	2	42	0	44	2	43	3554.8579	3554.85735	0.0006
106	1	39	4	35	0	40	4	36	3554.871	3554.87098	0
107	1	44	1	44	0	45	1	45	3554.8945	3554.8944	0.0001
108	1	36	5	31	0	37	5	32	3554.9057	3554.90548	0.0002
109	1	41	3	39	0	42	3	40	3554.9103	3554.91122	-0.0009
110	1	41	3	38	0	42	3	39	3554.9113	3554.91068	0.0006
111	1	44	0	44	0	45	0	45	3554.9187	3554.91926	-0.0006
112	1	43	1	42	0	44	1	43	3554.9808	3554.98108	-0.0003
113	1	42	2	40	0	43	2	41	3555.0053	3555.00588	-0.0006

114	1	42	2	41	0	43	2	42	3555.0169	3555.01775	-0.0008
115	1	32	6	26	0	33	6	27	3555.0328	3555.03297	-0.0002
116	1	38	4	34	0	39	4	35	3555.0395	3555.03892	0.0006
117	1	43	1	43	0	44	1	44	3555.0538	3555.05401	-0.0002
118	1	40	3	38	0	41	3	39	3555.0748	3555.07521	-0.0004
119	1	40	3	37	0	41	3	38	3555.0751	3555.07458	0.0005
120	1	43	0	43	0	44	0	44	3555.0784	3555.07876	-0.0004
121	1	35	5	30	0	36	5	31	3555.0794	3555.07931	0.0001
122	1	42	1	41	0	43	1	42	3555.1408	3555.1407	0.0001
123	1	41	2	39	0	42	2	40	3555.1669	3555.16725	-0.0003
124	1	41	2	40	0	42	2	41	3555.1797	3555.18005	-0.0004
125	1	37	4	33	0	38	4	34	3555.208	3555.20882	-0.0008
126	1	42	1	42	0	43	1	43	3555.215	3555.21543	-0.0004
127	1	31	6	25	0	32	6	26	3555.2152	3555.21462	0.0006
128	1	42	0	42	0	43	0	43	3555.2402	3555.24002	0.0002
129	1	39	3	37	0	40	3	38	3555.2402	3555.24116	-0.001
130	1	39	3	36	0	40	3	37	3555.2407	3555.24046	0.0002
131	1	34	5	29	0	35	5	30	3555.2559	3555.25509	0.0008
132	1	41	1	40	0	42	1	41	3555.3018	3555.30226	-0.0005
133	1	40	2	38	0	41	2	39	3555.3299	3555.33068	-0.0008
134	1	40	2	39	0	41	2	40	3555.3441	3555.34426	-0.0002
135	1	41	1	41	0	42	1	42	3555.3791	3555.37866	0.0004
136	1	36	4	32	0	37	4	33	3555.3817	3555.38067	0.001
137	1	41	0	41	0	42	0	42	3555.4027	3555.40306	-0.0004
138	1	38	3	35	0	39	3	36	3555.4083	3555.40833	0
139	1	38	3	36	0	39	3	37	3555.4084	3555.40906	-0.0007
140	1	33	5	28	0	34	5	29	3555.4337	3555.43282	0.0009
141	1	40	1	39	0	41	1	40	3555.4659	3555.46577	0.0001
142	1	39	2	37	0	40	2	38	3555.4957	3555.49617	-0.0005
143	1	39	2	38	0	40	2	39	3555.5104	3555.51037	0
144	1	40	1	40	0	41	1	41	3555.5436	3555.54371	-0.0001
145	1	35	4	31	0	36	4	32	3555.5535	3555.55447	-0.001
146	1	40	0	40	0	41	0	41	3555.5675	3555.56787	-0.0004
147	1	37	3	35	0	38	3	36	3555.5789	3555.57892	0
148	1	37	3	34	0	38	3	35	3555.5791	3555.57817	0.0009
149	1	32	5	27	0	33	5	28	3555.6118	3555.6125	-0.0007
150	1	39	1	38	0	40	1	39	3555.6306	3555.63123	-0.0006
151	1	38	2	36	0	39	2	37	3555.6633	3555.66373	-0.0004
152	1	38	2	37	0	39	2	38	3555.6784	3555.67839	0
153	1	39	1	39	0	40	1	40	3555.7102	3555.71058	-0.0004
154	1	34	4	30	0	35	4	31	3555.7311	3555.73023	0.0009
155	1	39	0	39	0	40	0	40	3555.7351	3555.73447	0.0006
156	1	36	3	33	0	37	3	34	3555.7496	3555.74998	-0.0004
157	1	36	3	34	0	37	3	35	3555.7504	3555.75074	-0.0003
158	1	31	5	26	0	32	5	27	3555.7936	3555.79411	-0.0005

159	1	38	1	37	0	39	1	38	3555.7993	3555.79865	0.0006
160	1	37	2	35	0	38	2	36	3555.8323	3555.83334	-0.001
161	1	37	2	36	0	38	2	37	3555.8482	3555.84832	-0.0001
162	1	38	1	38	0	39	1	39	3555.88	3555.87926	0.0007
163	1	38	0	38	0	39	0	39	3555.9039	3555.90285	0.001
164	1	33	4	29	0	34	4	30	3555.9084	3555.90793	0.0005
165	1	35	3	33	0	36	3	34	3555.9244	3555.92451	-0.0001
166	1	35	3	32	0	36	3	33	3555.9247	3555.92377	0.0009
167	1	37	1	36	0	38	1	37	3555.9675	3555.96805	-0.0005
168	1	30	5	25	0	31	5	26	3555.978	3555.97768	0.0003
169	1	36	2	34	0	37	2	35	3556.0044	3556.00501	-0.0006
170	1	36	2	35	0	37	2	36	3556.02	3556.02017	-0.0002
171	1	37	1	37	0	38	1	38	3556.049	3556.04977	-0.0008
172	1	37	0	37	0	38	0	38	3556.0733	3556.07303	0.0003
173	1	32	4	28	0	33	4	29	3556.0883	3556.08758	0.0007
174	1	34	3	31	0	35	3	32	3556.0987	3556.09952	-0.0008
175	1	34	3	32	0	35	3	33	3556.0992	3556.10023	-0.001
176	1	36	1	35	0	37	1	36	3556.1403	3556.13941	0.0009
177	1	29	5	24	0	30	5	25	3556.1626	3556.16318	-0.0006
178	1	35	2	33	0	36	2	34	3556.1781	3556.17872	-0.0006
179	1	35	2	34	0	36	2	35	3556.1941	3556.19393	0.0002
180	1	36	1	36	0	37	1	37	3556.2212	3556.2221	-0.0009
181	1	36	0	36	0	37	0	37	3556.2456	3556.24502	0.0006
182	1	31	4	27	0	32	4	28	3556.27	3556.26918	0.0008
183	1	33	3	31	0	34	3	32	3556.2772	3556.27791	-0.0007
184	1	33	3	30	0	34	3	31	3556.2774	3556.27723	0.0002
185	1	35	1	34	0	36	1	35	3556.3129	3556.31276	0.0001
186	1	28	5	23	0	29	5	24	3556.3514	3556.35063	0.0008
187	1	34	2	32	0	35	2	33	3556.3537	3556.35448	-0.0008
188	1	34	2	33	0	35	2	34	3556.3698	3556.36961	0.0002
189	1	35	1	35	0	36	1	36	3556.397	3556.39626	0.0007
190	1	35	0	35	0	36	0	36	3556.4188	3556.41881	0
191	1	30	4	26	0	31	4	27	3556.4522	3556.45273	-0.0005
192	1	32	3	29	0	33	3	30	3556.4575	3556.4569	0.0006
193	1	34	1	33	0	35	1	34	3556.4885	3556.4881	0.0004
194	1	33	2	31	0	34	2	32	3556.5325	3556.53226	0.0002
195	1	27	5	22	0	28	5	23	3556.5403	3556.54001	0.0003
196	1	33	2	32	0	34	2	33	3556.5472	3556.54722	0
197	1	34	1	34	0	35	1	35	3556.573	3556.57225	0.0008
198	1	34	0	34	0	35	0	35	3556.5936	3556.59443	-0.0008
199	1	29	4	25	0	30	4	26	3556.639	3556.63821	0.0008
200	1	31	3	28	0	32	3	29	3556.6392	3556.63852	0.0007
201	1	33	1	32	0	34	1	33	3556.6657	3556.66542	0.0003
202	1	32	2	30	0	33	2	31	3556.7117	3556.71207	-0.0004
203	1	32	2	31	0	33	2	32	3556.7263	3556.72674	-0.0004

204	1	26	5	21	0	27	5	22	3556.7315	3556.73134	0.0002
205	1	33	1	33	0	34	1	34	3556.7505	3556.75006	0.0004
206	1	33	0	33	0	34	0	34	3556.7725	3556.77188	0.0006
207	1	30	3	27	0	31	3	28	3556.8213	3556.82209	-0.0008
208	1	28	4	24	0	29	4	25	3556.8257	3556.82564	0.0001
209	1	32	1	31	0	33	1	32	3556.8445	3556.84474	-0.0002
210	1	31	2	29	0	32	2	30	3556.8931	3556.8939	-0.0008
211	1	31	2	30	0	32	2	31	3556.9088	3556.9082	0.0006
212	1	25	5	20	0	26	5	21	3556.9252	3556.9246	0.0006
213	1	32	1	32	0	33	1	33	3556.9299	3556.92971	0.0002
214	1	32	0	32	0	33	0	33	3556.9508	3556.95116	-0.0004
215	1	29	3	26	0	30	3	27	3557.0083	3557.00762	0.0007
216	1	27	4	23	0	28	4	24	3557.0153	3557.01502	0.0003
217	1	31	1	30	0	32	1	31	3557.0255	3557.02606	-0.0006
218	1	30	2	28	0	31	2	29	3557.0778	3557.07774	0.0001
219	1	30	2	29	0	31	2	30	3557.0924	3557.09157	0.0008
220	1	31	1	31	0	32	1	32	3557.1118	3557.1112	0.0006
221	1	24	5	19	0	25	5	20	3557.1206	3557.1198	0.0008
222	1	31	0	31	0	32	0	32	3557.133	3557.13229	0.0007
223	1	28	3	25	0	29	3	26	3557.1943	3557.19509	-0.0008
224	1	26	4	22	0	27	4	23	3557.2053	3557.20633	-0.001
225	1	30	1	29	0	31	1	30	3557.2102	3557.20938	0.0008
226	1	29	2	27	0	30	2	28	3557.2645	3557.26357	0.0009
227	1	29	2	28	0	30	2	29	3557.2766	3557.27688	-0.0003
228	1	30	1	30	0	31	1	31	3557.2941	3557.29452	-0.0004
229	1	30	0	30	0	31	0	31	3557.3153	3557.31529	0
230	1	23	5	18	0	24	5	19	3557.317	3557.31693	0.0001
231	1	27	3	24	0	28	3	25	3557.3852	3557.3845	0.0007
232	1	29	1	28	0	30	1	29	3557.3944	3557.39471	-0.0003
233	1	25	4	21	0	26	4	22	3557.3997	3557.39958	0.0001
234	1	28	2	26	0	29	2	27	3557.452	3557.45139	0.0006
235	1	28	2	27	0	29	2	28	3557.4632	3557.46411	-0.0009
236	1	29	1	29	0	30	1	30	3557.4793	3557.47968	-0.0004
237	1	29	0	29	0	30	0	30	3557.501	3557.50015	0.0009
238	1	22	5	17	0	23	5	18	3557.5163	3557.51599	0.0003
239	1	26	3	23	0	27	3	24	3557.5755	3557.57585	-0.0004
240	1	28	1	27	0	29	1	28	3557.5823	3557.58204	0.0003
241	1	24	4	20	0	25	4	21	3557.5946	3557.59476	-0.0002
242	1	27	2	25	0	28	2	26	3557.6414	3557.6412	0.0002
243	1	27	2	26	0	28	2	27	3557.6524	3557.65328	-0.0009
244	1	28	1	28	0	29	1	29	3557.6664	3557.66668	-0.0003
245	1	28	0	28	0	29	0	29	3557.6868	3557.68688	-0.0001
246	1	21	5	16	0	22	5	17	3557.7164	3557.71699	-0.0006
247	1	11	11	0	0	11	11	1	3557.7537	3557.75327	0.0004
248	1	25	3	22	0	26	3	23	3557.7683	3557.76914	-0.0008

249	1	27	1	26	0	28	1	27	3557.7716	3557.77139	0.0002
250	1	12	11	1	0	12	11	2	3557.7756	3557.776	-0.0004
251	1	23	4	19	0	24	4	20	3557.7919	3557.79188	0
252	1	13	11	2	0	13	11	3	3557.8015	3557.80062	0.0009
253	1	14	11	3	0	14	11	4	3557.8271	3557.82713	0
254	1	26	2	24	0	27	2	25	3557.834	3557.83298	0.001
255	1	26	2	25	0	27	2	26	3557.8433	3557.84437	-0.0011
256	1	27	1	27	0	28	1	28	3557.8553	3557.85552	-0.0002
257	1	15	11	4	0	15	11	5	3557.8556	3557.85553	0.0001
258	1	27	0	27	0	28	0	28	3557.8752	3557.87551	-0.0003
259	1	16	11	5	0	16	11	6	3557.8856	3557.88582	-0.0002
260	1	17	11	6	0	17	11	7	3557.9175	3557.918	-0.0005
261	1	20	5	15	0	21	5	16	3557.9194	3557.91992	-0.0005
262	1	18	11	7	0	18	11	8	3557.9512	3557.95206	-0.0009
263	1	26	1	25	0	27	1	26	3557.9627	3557.96275	-0.0001
264	1	24	3	21	0	25	3	22	3557.964	3557.96437	-0.0004
265	1	19	11	8	0	19	11	9	3557.9875	3557.98801	-0.0005
266	1	22	4	18	0	23	4	19	3557.9915	3557.99094	0.0006
267	1	25	2	23	0	26	2	24	3558.0262	3558.02672	-0.0005
268	1	25	2	24	0	26	2	25	3558.0379	3558.0374	0.0005
269	1	26	1	26	0	27	1	27	3558.0456	3558.0462	-0.0006
270	1	26	0	26	0	27	0	27	3558.0663	3558.06603	0.0003
271	1	19	5	14	0	20	5	15	3558.1244	3558.12478	-0.0004
272	1	25	1	24	0	26	1	25	3558.1564	3558.15613	0.0003
273	1	23	3	20	0	24	3	21	3558.1618	3558.16153	0.0003
274	1	21	4	17	0	22	4	18	3558.1916	3558.19192	-0.0003
275	1	24	2	22	0	25	2	23	3558.2222	3558.22242	-0.0002
276	1	24	2	23	0	25	2	24	3558.2316	3558.23236	-0.0008
277	1	25	1	25	0	26	1	26	3558.2383	3558.23872	-0.0004
278	1	25	0	25	0	26	0	26	3558.2587	3558.25845	0.0002
279	1	18	5	13	0	19	5	14	3558.3316	3558.33157	0
280	1	24	1	23	0	25	1	24	3558.3515	3558.35153	0
281	1	22	3	19	0	23	3	20	3558.3602	3558.36062	-0.0004
282	1	20	4	16	0	21	4	17	3558.3945	3558.39484	-0.0003
283	1	23	2	21	0	24	2	22	3558.4197	3558.42006	-0.0004
284	1	23	2	22	0	24	2	23	3558.4283	3558.42925	-0.001
285	1	24	1	24	0	25	1	25	3558.4331	3558.4331	0
286	1	24	0	24	0	25	0	25	3558.4519	3558.45279	-0.0009
287	1	17	5	12	0	18	5	13	3558.54	3558.54028	-0.0003
288	1	23	1	22	0	24	1	23	3558.5483	3558.54894	-0.0006
289	1	21	3	18	0	22	3	19	3558.5615	3558.56164	-0.0001
290	1	19	4	15	0	20	4	16	3558.5992	3558.59969	-0.0005
291	1	22	2	20	0	23	2	21	3558.619	3558.61964	-0.0006
292	1	22	2	21	0	23	2	22	3558.6271	3558.62808	-0.001
293	1	23	1	23	0	24	1	24	3558.629	3558.62931	-0.0003



294	1	23	0	23	0	24	0	24	3558.6498	3558.64905	0.0007
295	1	22	1	21	0	23	1	22	3558.7483	3558.74838	-0.0001
296	1	16	5	11	0	17	5	12	3558.7516	3558.75092	0.0007
297	1	20	3	17	0	21	3	18	3558.7651	3558.76459	0.0005
298	1	18	4	14	0	19	4	15	3558.8063	3558.80646	-0.0002
299	1	10	10	1	0	10	10	0	3558.8148	3558.81546	-0.0007
300	1	10	10	0	0	10	10	1	3558.8151	3558.81546	-0.0004
301	1	22	1	22	0	23	1	23	3558.8273	3558.82738	-0.0001
302	1	21	2	20	0	22	2	21	3558.8299	3558.82884	0.0011
303	1	11	10	1	0	11	10	2	3558.8362	3558.83629	-0.0001
304	1	11	10	2	0	11	10	1	3558.8372	3558.83629	0.0009
305	1	22	0	22	0	23	0	23	3558.8474	3558.84725	0.0002
306	1	12	10	3	0	12	10	2	3558.8585	3558.85902	-0.0005
307	1	12	10	2	0	12	10	3	3558.8585	3558.85902	-0.0005
308	1	13	10	4	0	13	10	3	3558.8833	3558.88363	-0.0003
309	1	13	10	3	0	13	10	4	3558.8846	3558.88363	0.001
310	1	21	1	20	0	22	1	21	3558.9507	3558.94984	0.0009
311	1	19	3	16	0	20	3	17	3558.9688	3558.96947	-0.0007
312	1	17	4	13	0	18	4	14	3559.0143	3559.01516	-0.0009
313	1	21	1	21	0	22	1	22	3559.027	3559.02729	-0.0003
314	1	20	2	19	0	21	2	20	3559.0309	3559.03154	-0.0006
315	1	21	0	21	0	22	0	22	3559.0482	3559.04737	0.0008
316	1	20	1	19	0	21	1	20	3559.1538	3559.15332	0.0005
317	1	18	3	15	0	19	3	16	3559.1756	3559.17627	-0.0007
318	1	16	4	12	0	17	4	13	3559.2259	3559.22578	0.0001
319	1	20	1	20	0	21	1	21	3559.2286	3559.22906	-0.0005
320	1	19	2	18	0	20	2	19	3559.2372	3559.23617	0.001
321	1	20	0	20	0	21	0	21	3559.2498	3559.24944	0.0004
322	1	19	1	18	0	20	1	19	3559.3594	3559.35882	0.0006
323	1	17	3	14	0	18	3	15	3559.3851	3559.38499	0.0001
324	1	19	1	19	0	20	1	20	3559.4329	3559.43267	0.0002
325	1	15	4	11	0	16	4	12	3559.4383	3559.43832	0
326	1	18	2	17	0	19	2	18	3559.4426	3559.44274	-0.0001
327	1	19	0	19	0	20	0	20	3559.4537	3559.45346	0.0002
328	1	18	1	17	0	19	1	18	3559.566	3559.56635	-0.0003
329	1	16	3	13	0	17	3	14	3559.5958	3559.59563	0.0002
330	1	18	1	18	0	19	1	19	3559.6375	3559.63813	-0.0006
331	1	17	2	16	0	18	2	17	3559.6511	3559.65123	-0.0001
332	1	14	4	10	0	15	4	11	3559.6522	3559.65279	-0.0006
333	1	18	0	18	0	19	0	19	3559.6597	3559.65943	0.0003
334	1	17	1	16	0	18	1	17	3559.776	3559.7759	0.0001
335	1	9	9	0	0	9	9	1	3559.7815	3559.7812	0.0003
336	1	10	9	1	0	10	9	2	3559.8001	3559.80014	0
337	1	15	3	12	0	16	3	13	3559.8084	3559.80819	0.0002
338	1	11	9	2	0	11	9	3	3559.8213	3559.82098	0.0003

339	1	12	9	3	0	12	9	4	3559.8446	3559.8437	0.0009
340	1	17	1	17	0	18	1	18	3559.8456	3559.84544	0.0002
341	1	16	2	15	0	17	2	16	3559.862	3559.86166	0.0003
342	1	17	0	17	0	18	0	18	3559.8667	3559.86736	-0.0007
343	1	13	9	4	0	13	9	5	3559.8689	3559.86832	0.0006
344	1	13	4	9	0	14	4	10	3559.8693	3559.86918	0.0001
345	1	14	9	5	0	14	9	6	3559.8953	3559.89482	0.0005
346	1	15	9	6	0	15	9	7	3559.9229	3559.92322	-0.0003
347	1	16	1	15	0	17	1	16	3559.9875	3559.98747	0
348	1	14	3	11	0	15	3	12	3560.0225	3560.02267	-0.0002
349	1	16	1	16	0	17	1	17	3560.0539	3560.0546	-0.0007
350	1	15	2	14	0	16	2	15	3560.0748	3560.07402	0.0008
351	1	16	0	16	0	17	0	17	3560.0771	3560.07725	-0.0002
352	1	12	4	8	0	13	4	9	3560.0876	3560.08748	0.0001
353	1	15	1	14	0	16	1	15	3560.2003	3560.20106	-0.0008
354	1	13	3	10	0	14	3	11	3560.2394	3560.23907	0.0003
355	1	15	1	15	0	16	1	16	3560.2654	3560.26561	-0.0002
356	1	14	2	13	0	15	2	14	3560.2884	3560.28832	0.0001
357	1	15	0	15	0	16	0	16	3560.2891	3560.28911	0
358	1	11	4	7	0	12	4	8	3560.308	3560.3077	0.0003
359	1	14	1	13	0	15	1	14	3560.4158	3560.41667	-0.0009
360	1	12	3	9	0	13	3	10	3560.4567	3560.45737	-0.0007
361	1	14	1	14	0	15	1	15	3560.4778	3560.47847	-0.0007
362	1	14	0	14	0	15	0	15	3560.5037	3560.50293	0.0008
363	1	10	4	6	0	11	4	7	3560.5306	3560.52983	0.0008
364	1	8	8	0	0	8	8	1	3560.6491	3560.64906	0
365	1	9	8	1	0	9	8	2	3560.6652	3560.66611	-0.0009
366	1	11	3	8	0	12	3	9	3560.678	3560.6776	0.0004
367	1	10	8	2	0	10	8	3	3560.6847	3560.68505	-0.0004
368	1	11	8	3	0	11	8	4	3560.7064	3560.70588	0.0005
369	1	12	8	4	0	12	8	5	3560.7297	3560.72861	0.0011
370	1	13	8	5	0	13	8	6	3560.7534	3560.75322	0.0002
371	1	9	4	5	0	10	4	6	3560.7539	3560.75388	0
372	1	14	8	6	0	14	8	7	3560.7797	3560.77973	0
373	1	7	7	0	0	7	7	1	3561.418	3561.41775	0.0002
374	1	8	7	1	0	8	7	2	3561.4319	3561.43291	-0.001
375	1	9	7	2	0	9	7	3	3561.4507	3561.44995	0.0007
376	1	10	7	3	0	10	7	4	3561.4686	3561.46889	-0.0003
377	1	11	7	4	0	11	7	5	3561.4897	3561.48972	0
378	1	12	7	5	0	12	7	6	3561.5126	3561.51245	0.0002
379	1	13	7	6	0	13	7	7	3561.5378	3561.53706	0.0007
380	1	14	7	7	0	14	7	8	3561.563	3561.56357	-0.0006
381	1	6	6	0	0	6	6	1	3562.086	3562.08613	-0.0001
382	1	7	6	1	0	7	6	2	3562.0992	3562.09939	-0.0002
383	1	8	6	2	0	8	6	3	3562.1146	3562.11454	0.0001

384	1	9	6	3	0	9	6	4	3562.1306	3562.13159	-0.001
385	1	10	6	4	0	10	6	5	3562.1497	3562.15052	-0.0008
386	1	11	6	5	0	11	6	6	3562.1709	3562.17136	-0.0005
387	1	12	6	6	0	12	6	7	3562.1946	3562.19408	0.0005
388	1	13	6	7	0	13	6	8	3562.2187	3562.2187	0
389	1	14	6	8	0	14	6	9	3562.2453	3562.2452	0.0001
390	1	15	6	9	0	15	6	10	3562.2743	3562.2736	0.0007
391	1	16	6	10	0	16	6	11	3562.3043	3562.30389	0.0004
392	1	17	6	11	0	17	6	12	3562.335	3562.33607	-0.0011
393	1	18	6	12	0	18	6	13	3562.3705	3562.37014	0.0004
394	1	19	6	13	0	19	6	14	3562.4067	3562.40609	0.0006
395	1	20	6	14	0	20	6	15	3562.4442	3562.44394	0.0003
396	1	21	6	15	0	21	6	16	3562.4839	3562.48367	0.0002
397	1	22	6	16	0	22	6	17	3562.5247	3562.52529	-0.0006
398	1	5	5	0	0	5	5	1	3562.653	3562.6532	-0.0002
399	1	6	5	1	0	6	5	2	3562.6648	3562.66457	0.0002
400	1	7	5	2	0	7	5	3	3562.6771	3562.67783	-0.0007
401	1	8	5	3	0	8	5	4	3562.693	3562.69298	0
402	1	4	4	0	0	4	4	1	3563.1184	3563.11814	0.0003
403	1	5	4	1	0	5	4	2	3563.1268	3563.12761	-0.0008
404	1	6	4	2	0	6	4	3	3563.1379	3563.13897	-0.0011
405	1	7	4	3	0	7	4	4	3563.153	3563.15223	0.0008
406	1	8	4	4	0	8	4	5	3563.168	3563.16739	0.0006
407	1	9	4	5	0	9	4	6	3563.1849	3563.18444	0.0005
408	1	10	4	6	0	10	4	7	3563.2039	3563.20338	0.0005
409	1	6	5	1	0	5	5	0	3564.1231	3564.1232	-0.0001
410	1	2	1	2	0	1	1	1	3564.3785	3564.37833	0.0002
411	1	7	5	2	0	6	5	1	3564.3787	3564.37954	-0.0008
412	1	2	1	1	0	1	1	0	3564.3892	3564.38944	-0.0002
413	1	3	2	1	0	2	2	0	3564.4736	3564.47384	-0.0002
414	1	6	4	2	0	5	4	1	3564.5973	3564.59742	-0.0001
415	1	8	5	3	0	7	5	2	3564.6371	3564.63776	-0.0007
416	1	3	1	2	0	2	1	1	3564.6404	3564.64104	-0.0006
417	1	5	3	2	0	4	3	1	3564.712	3564.71257	-0.0006
418	1	4	2	3	0	3	2	2	3564.7251	3564.7244	0.0007
419	1	7	4	3	0	6	4	2	3564.8528	3564.85373	-0.0009
420	1	4	1	3	0	3	1	2	3564.8952	3564.8946	0.0006
421	1	9	5	4	0	8	5	3	3564.8971	3564.89785	-0.0008
422	1	6	3	3	0	5	3	2	3564.9664	3564.96698	-0.0006
423	1	5	2	4	0	4	2	3	3564.9766	3564.97687	-0.0003
424	1	8	4	4	0	7	4	3	3565.1115	3565.11192	-0.0004
425	1	5	1	5	0	4	1	4	3565.1205	3565.1211	-0.0006
426	1	5	1	4	0	4	1	3	3565.1497	3565.15013	-0.0004
427	1	10	5	5	0	9	5	4	3565.1607	3565.15982	0.0009
428	1	7	3	4	0	6	3	3	3565.2238	3565.22327	0.0005

429	1	6	2	5	0	5	2	4	3565.2318	3565.23122	0.0006
430	1	9	4	5	0	8	4	4	3565.3711	3565.37199	-0.0009
431	1	6	1	6	0	5	1	5	3565.3732	3565.37228	0.0009
432	1	6	1	5	0	5	1	4	3565.4069	3565.4076	-0.0007
433	1	11	5	6	0	10	5	5	3565.4237	3565.42367	0
434	1	8	3	5	0	7	3	4	3565.4824	3565.48145	0.001
435	1	7	2	6	0	6	2	5	3565.4879	3565.48743	0.0005
436	1	7	1	7	0	6	1	6	3565.6251	3565.62523	-0.0001
437	1	10	4	6	0	9	4	5	3565.6342	3565.63394	0.0003
438	1	7	1	6	0	6	1	5	3565.6678	3565.66702	0.0008
439	1	12	5	7	0	11	5	6	3565.6894	3565.68938	0
440	1	9	3	6	0	8	3	5	3565.7424	3565.74151	0.0009
441	1	8	2	7	0	7	2	6	3565.7459	3565.74552	0.0004
442	1	8	1	8	0	7	1	7	3565.8806	3565.87996	0.0006
443	1	11	4	7	0	10	4	6	3565.8984	3565.89776	0.0006
444	1	8	1	7	0	7	1	6	3565.9277	3565.92838	-0.0007
445	1	13	5	8	0	12	5	7	3565.9559	3565.95697	-0.0011
446	1	10	3	7	0	9	3	6	3566.0026	3566.00346	-0.0009
447	1	9	2	8	0	8	2	7	3566.0053	3566.00546	-0.0002
448	1	9	1	9	0	8	1	8	3566.1359	3566.13646	-0.0006
449	1	12	4	8	0	11	4	7	3566.1641	3566.16346	0.0006
450	1	9	1	8	0	8	1	7	3566.1925	3566.19168	0.0008
451	1	14	5	9	0	13	5	8	3566.2265	3566.22642	0.0001
452	1	10	2	9	0	9	2	8	3566.267	3566.26726	-0.0003
453	1	11	3	8	0	10	3	7	3566.267	3566.2673	-0.0003
454	1	10	1	10	0	9	1	9	3566.3939	3566.39472	-0.0008
455	1	13	4	9	0	12	4	8	3566.4314	3566.43103	0.0004
456	1	10	1	9	0	9	1	8	3566.4573	3566.45691	0.0004
457	1	15	5	10	0	14	5	9	3566.497	3566.49774	-0.0007
458	1	11	2	10	0	10	2	9	3566.5303	3566.5309	-0.0006
459	1	12	3	9	0	11	3	8	3566.5337	3566.53301	0.0007
460	1	11	1	11	0	10	1	10	3566.6556	3566.65475	0.0009
461	1	14	4	10	0	13	4	9	3566.7001	3566.70047	-0.0004
462	1	11	1	10	0	10	1	9	3566.7242	3566.72406	0.0001
463	1	16	5	11	0	15	5	10	3566.7702	3566.77092	-0.0007
464	1	12	2	11	0	11	2	10	3566.7957	3566.79639	-0.0007
465	1	13	3	10	0	12	3	9	3566.8007	3566.80061	0.0001
466	1	12	1	12	0	11	1	11	3566.9169	3566.91652	0.0004
467	1	15	4	11	0	14	4	10	3566.9718	3566.97179	0
468	1	12	1	11	0	11	1	10	3566.9938	3566.99312	0.0007
469	1	13	2	12	0	12	2	11	3567.064	3567.06373	0.0003
470	1	14	3	11	0	13	3	10	3567.0707	3567.0701	0.0006
471	1	13	1	13	0	12	1	12	3567.1805	3567.18005	0.0005
472	1	16	4	12	0	15	4	11	3567.2458	3567.24497	0.0008
473	1	13	1	12	0	12	1	11	3567.2643	3567.26409	0.0002

474	1	14	2	13	0	13	2	12	3567.3328	3567.33289	-0.0001
475	1	15	3	12	0	14	3	11	3567.3422	3567.34146	0.0007
476	1	14	1	14	0	13	1	13	3567.4462	3567.44531	0.0009
477	1	15	2	14	0	14	2	13	3567.6043	3567.60388	0.0004
478	1	16	3	13	0	15	3	12	3567.6148	3567.6147	0.0001
479	1	17	3	14	0	16	3	13	3567.8908	3567.88983	0.001
480	1	18	3	15	0	17	3	14	3568.1672	3568.16684	0.0004
481	1	19	3	16	0	18	3	15	3568.4452	3568.44573	-0.0005
482	1	32	6	26	0	31	6	25	3570.8158	3570.81503	0.0008
483	1	33	6	27	0	32	6	26	3571.1196	3571.11943	0.0002
484	1	34	6	28	0	33	6	27	3571.4256	3571.42563	0
485	1	35	6	29	0	34	6	28	3571.7331	3571.73364	-0.0005
486	1	36	6	30	0	35	6	29	3572.0444	3572.04346	0.0009
487	1	37	6	31	0	36	6	30	3572.3549	3572.35507	-0.0002
488	1	48	8	40	0	47	8	39	3574.4358	3574.43644	-0.0006
489	1	49	8	41	0	48	8	40	3574.7698	3574.7692	0.0006
490	1	50	8	42	0	49	8	41	3575.1034	3575.10369	-0.0003
491	1	42	3	40	0	41	3	39	3575.3687	3575.36847	0.0002
492	1	51	8	43	0	50	8	42	3575.4398	3575.43992	-0.0001
493	1	43	3	41	0	42	3	40	3575.691	3575.69122	-0.0002
494	1	43	3	40	0	42	3	39	3575.7086	3575.70808	0.0005
495	1	52	8	44	0	51	8	43	3575.7781	3575.77788	0.0002
496	1	50	7	43	0	49	7	42	3575.8873	3575.88635	0.0009
497	1	44	3	42	0	43	3	41	3576.0163	3576.01573	0.0006
498	1	44	3	41	0	43	3	40	3576.0357	3576.03477	0.0009
499	1	53	8	45	0	52	8	44	3576.1175	3576.11757	-0.0001
500	1	47	5	42	0	46	5	41	3576.1494	3576.14928	0.0001
501	1	51	7	44	0	50	7	43	3576.2231	3576.22264	0.0005
502	1	45	3	43	0	44	3	42	3576.3424	3576.34199	0.0004
503	1	45	3	42	0	44	3	41	3576.3643	3576.36345	0.0009
504	1	54	8	46	0	53	8	45	3576.4597	3576.45897	0.0007
505	1	48	5	43	0	47	5	42	3576.4813	3576.48066	0.0006
506	1	52	7	45	0	51	7	44	3576.5612	3576.56066	0.0005
507	1	46	3	44	0	45	3	43	3576.6706	3576.67001	0.0006
508	1	46	3	43	0	45	3	42	3576.695	3576.69411	0.0009
509	1	55	8	47	0	54	8	46	3576.8028	3576.80209	0.0007
510	1	49	5	44	0	48	5	43	3576.8145	3576.81381	0.0007
511	1	53	7	46	0	52	7	45	3576.8998	3576.90041	-0.0006
512	1	48	4	44	0	47	4	43	3576.9609	3576.96128	-0.0004
513	1	47	3	45	0	46	3	44	3576.9987	3576.99976	-0.0011
514	1	47	3	44	0	46	3	43	3577.0276	3577.02676	0.0008
515	1	56	8	48	0	55	8	47	3577.1464	3577.14692	-0.0005
516	1	50	5	45	0	49	5	44	3577.1486	3577.14873	-0.0001
517	1	47	2	46	0	46	2	45	3577.1988	3577.19908	-0.0003
518	1	54	7	47	0	53	7	46	3577.2416	3577.24188	-0.0003

519	1	52	6	46	0	51	6	45	3577.2431	3577.24263	0.0005
520	1	49	4	45	0	48	4	44	3577.2948	3577.29504	-0.0002
521	1	48	3	46	0	47	3	45	3577.3313	3577.33125	0.0001
522	1	48	3	45	0	47	3	44	3577.3617	3577.36141	0.0003
523	1	47	2	45	0	46	2	44	3577.4122	3577.41172	0.0005
524	1	51	5	46	0	50	5	45	3577.4855	3577.48541	0.0001
525	1	57	8	49	0	56	8	48	3577.4945	3577.49345	0.001
526	1	48	2	47	0	47	2	46	3577.5262	3577.52629	-0.0001
527	1	53	6	47	0	52	6	46	3577.5824	3577.58253	-0.0001
528	1	55	7	48	0	54	7	47	3577.5848	3577.58508	-0.0003
529	1	50	4	46	0	49	4	45	3577.6296	3577.63061	-0.001
530	1	49	3	47	0	48	3	46	3577.6637	3577.66446	-0.0008
531	1	49	3	46	0	48	3	45	3577.6971	3577.69807	-0.001
532	1	48	2	46	0	47	2	45	3577.7513	3577.75134	0
533	1	49	1	49	0	48	1	48	3577.7735	3577.77426	-0.0008
534	1	52	5	47	0	51	5	46	3577.8241	3577.82385	0.0002
535	1	58	8	50	0	57	8	49	3577.8416	3577.84169	-0.0001
536	1	49	2	48	0	48	2	47	3577.8559	3577.85506	0.0008
537	1	54	6	48	0	53	6	47	3577.9235	3577.92416	-0.0007
538	1	56	7	49	0	55	7	48	3577.9302	3577.92999	0.0002
539	1	51	4	48	0	50	4	47	3577.9668	3577.96591	0.0009
540	1	51	4	47	0	50	4	46	3577.9675	3577.96799	-0.0005
541	1	50	3	48	0	49	3	47	3578.0001	3577.99939	0.0007
542	1	50	3	47	0	49	3	46	3578.0375	3578.03674	0.0008
543	1	49	2	47	0	48	2	46	3578.0934	3578.09277	0.0006
544	1	50	1	50	0	49	1	49	3578.0968	3578.09781	-0.001
545	1	53	5	48	0	52	5	47	3578.1649	3578.16405	0.0008
546	1	50	2	49	0	49	2	48	3578.1854	3578.18538	0
547	1	59	8	51	0	58	8	50	3578.1911	3578.19162	-0.0005
548	1	49	1	48	0	48	1	47	3578.198	3578.1977	0.0003
549	1	55	6	49	0	54	6	48	3578.2673	3578.26752	-0.0002
550	1	57	7	50	0	56	7	49	3578.2771	3578.27662	0.0005
551	1	52	4	49	0	51	4	48	3578.3054	3578.30479	0.0006
552	1	52	4	48	0	51	4	47	3578.3077	3578.30718	0.0005
553	1	51	3	49	0	50	3	48	3578.3365	3578.33602	0.0005
554	1	51	3	48	0	50	3	47	3578.3777	3578.37744	0.0003
555	1	51	1	51	0	50	1	50	3578.4227	3578.42288	-0.0002
556	1	50	2	48	0	49	2	47	3578.4362	3578.436	0.0002
557	1	54	5	49	0	53	5	48	3578.5066	3578.506	0.0006
558	1	51	2	50	0	50	2	49	3578.5168	3578.51724	-0.0004
559	1	50	1	49	0	49	1	48	3578.5316	3578.53061	0.001
560	1	60	8	52	0	59	8	51	3578.5436	3578.54325	0.0004
561	1	56	6	50	0	55	6	49	3578.6131	3578.61261	0.0005
562	1	58	7	51	0	57	7	50	3578.6257	3578.62496	0.0007
563	1	53	4	50	0	52	4	49	3578.6461	3578.64542	0.0007

564	1	53	4	49	0	52	4	48	3578.6475	3578.64818	-0.0007
565	1	52	3	50	0	51	3	49	3578.6745	3578.67435	0.0002
566	1	52	3	49	0	51	3	48	3578.7196	3578.72016	-0.0006
567	1	52	1	52	0	51	1	51	3578.7501	3578.74945	0.0007
568	1	51	2	49	0	50	2	48	3578.7813	3578.78099	0.0003
569	1	55	5	50	0	54	5	49	3578.8488	3578.8497	-0.0009
570	1	52	2	51	0	51	2	50	3578.851	3578.85062	0.0004
571	1	51	1	50	0	50	1	49	3578.8654	3578.86485	0.0005
572	1	61	8	53	0	60	8	52	3578.8963	3578.89656	-0.0003
573	1	57	6	51	0	56	6	50	3578.9596	3578.95943	0.0002
574	1	59	7	52	0	58	7	51	3578.9747	3578.975	-0.0003
575	1	54	4	51	0	53	4	50	3578.987	3578.98783	-0.0008
576	1	54	4	50	0	53	4	49	3578.9904	3578.99099	-0.0006
577	1	53	3	51	0	52	3	50	3579.0142	3579.01437	-0.0002
578	1	53	3	50	0	52	3	49	3579.0644	3579.06492	-0.0005
579	1	53	1	53	0	52	1	52	3579.0785	3579.07752	0.001
580	1	52	2	50	0	51	2	49	3579.1275	3579.12772	-0.0002
581	1	53	2	52	0	52	2	51	3579.1854	3579.18554	-0.0001
582	1	56	5	51	0	55	5	50	3579.1946	3579.19515	-0.0005
583	1	52	1	51	0	51	1	50	3579.2014	3579.20041	0.001
584	1	62	8	54	0	61	8	53	3579.2507	3579.25156	-0.0009
585	1	58	6	52	0	57	6	51	3579.3085	3579.30796	0.0005
586	1	60	7	53	0	59	7	52	3579.3262	3579.32674	-0.0005
587	1	55	4	52	0	54	4	51	3579.3323	3579.33199	0.0003
588	1	55	4	51	0	54	4	50	3579.3347	3579.33561	-0.0009
589	1	54	3	52	0	53	3	51	3579.3552	3579.35606	-0.0009
590	1	54	1	54	0	53	1	53	3579.4069	3579.4071	-0.0002
591	1	54	3	51	0	53	3	50	3579.4124	3579.41173	0.0007
592	1	53	2	51	0	52	2	50	3579.4759	3579.47616	-0.0003
593	1	54	2	53	0	53	2	52	3579.5222	3579.52196	0.0002
594	1	53	1	52	0	52	1	51	3579.5375	3579.53726	0.0002
595	1	57	5	52	0	56	5	51	3579.5421	3579.54234	-0.0002
596	1	63	8	55	0	62	8	54	3579.6087	3579.60823	0.0005
597	1	59	6	53	0	58	6	52	3579.6575	3579.65821	-0.0007
598	1	56	4	53	0	55	4	52	3579.6782	3579.6779	0.0003
599	1	61	7	54	0	60	7	53	3579.6798	3579.68017	-0.0004
600	1	56	4	52	0	55	4	51	3579.682	3579.68203	0
601	1	55	3	53	0	54	3	52	3579.6989	3579.69942	-0.0005
602	1	55	1	55	0	54	1	54	3579.7393	3579.73817	0.0011
603	1	55	3	52	0	54	3	51	3579.7607	3579.76059	0.0001
604	1	54	2	52	0	53	2	51	3579.8262	3579.82628	-0.0001
605	1	55	2	54	0	54	2	53	3579.8607	3579.85989	0.0008
606	1	54	1	53	0	53	1	52	3579.8746	3579.87537	-0.0008
607	1	58	5	53	0	57	5	52	3579.8914	3579.89127	0.0001
608	1	64	8	56	0	63	8	55	3579.9669	3579.96657	0.0003

609	1	57	4	54	0	56	4	53	3580.0251	3580.02556	-0.0005
610	1	57	4	53	0	56	4	52	3580.0299	3580.03027	-0.0004
611	1	62	7	55	0	61	7	54	3580.0357	3580.03529	0.0004
612	1	56	3	54	0	55	3	53	3580.0438	3580.04444	-0.0006
613	1	56	1	56	0	55	1	55	3580.0706	3580.07073	-0.0001
614	1	56	3	53	0	55	3	52	3580.1106	3580.1115	-0.0009
615	1	55	2	53	0	54	2	52	3580.1788	3580.17806	0.0007
616	1	56	2	55	0	55	2	54	3580.1998	3580.19931	0.0005
617	1	55	1	54	0	54	1	53	3580.2143	3580.21473	-0.0004
618	1	59	5	54	0	58	5	53	3580.2423	3580.24194	0.0004
619	1	58	4	55	0	57	4	54	3580.3741	3580.37497	-0.0009
620	1	58	4	54	0	57	4	53	3580.3799	3580.38032	-0.0004
621	1	57	3	55	0	56	3	54	3580.3901	3580.39111	-0.001
622	1	63	7	56	0	62	7	55	3580.3921	3580.3921	0
623	1	57	1	57	0	56	1	56	3580.4053	3580.40478	0.0005
624	1	57	3	54	0	56	3	53	3580.4646	3580.46447	0.0001
625	1	56	2	54	0	55	2	53	3580.5305	3580.53147	-0.001
626	1	57	2	56	0	56	2	55	3580.5393	3580.54022	-0.0009
627	1	56	1	55	0	55	1	54	3580.5561	3580.55531	0.0008
628	1	60	5	55	0	59	5	54	3580.5941	3580.59433	-0.0002
629	1	62	6	56	0	61	6	55	3580.7192	3580.7192	0
630	1	59	4	56	0	58	4	55	3580.7264	3580.72612	0.0003
631	1	59	4	55	0	58	4	54	3580.733	3580.73217	0.0008
632	1	58	3	56	0	57	3	55	3580.7385	3580.73941	-0.0009
633	1	58	1	58	0	57	1	57	3580.7401	3580.74031	-0.0002
634	1	64	7	57	0	63	7	56	3580.7507	3580.75059	0.0001
635	1	58	3	55	0	57	3	54	3580.8203	3580.81951	0.0008
636	1	58	2	57	0	57	2	56	3580.8824	3580.8826	-0.0002
637	1	57	2	55	0	56	2	54	3580.8859	3580.88649	-0.0006
638	1	57	1	56	0	56	1	55	3580.8973	3580.8971	0.0002
639	1	61	5	56	0	60	5	55	3580.9479	3580.94846	-0.0006
640	1	59	1	59	0	58	1	58	3581.077	3581.07732	-0.0003
641	1	60	4	57	0	59	4	56	3581.0792	3581.07899	0.0002
642	1	60	4	56	0	59	4	55	3581.0859	3581.08584	0.0001
643	1	59	3	57	0	58	3	56	3581.0895	3581.08934	0.0002
644	1	59	3	56	0	58	3	55	3581.1771	3581.17661	0.0005
645	1	59	2	58	0	58	2	57	3581.2271	3581.22645	0.0006
646	1	58	1	57	0	57	1	56	3581.24	3581.24008	-0.0001
647	1	58	2	56	0	57	2	55	3581.2425	3581.24309	-0.0006
648	1	60	1	60	0	59	1	59	3581.4153	3581.41581	-0.0005
649	1	61	4	58	0	60	4	57	3581.4336	3581.4336	0
650	1	60	3	58	0	59	3	57	3581.4404	3581.44089	-0.0005
651	1	61	4	57	0	60	4	56	3581.4406	3581.44132	-0.0007
652	1	60	3	57	0	59	3	56	3581.5363	3581.53578	0.0005
653	1	60	2	59	0	59	2	58	3581.5727	3581.57177	0.0009



654	1	59	1	58	0	58	1	57	3581.5849	3581.58422	0.0007
655	1	59	2	57	0	58	2	56	3581.6007	3581.60124	-0.0005
656	1	61	1	61	0	60	1	60	3581.7566	3581.75577	0.0008
657	1	62	4	59	0	61	4	58	3581.7891	3581.78992	-0.0008
658	1	61	3	59	0	60	3	58	3581.7947	3581.79403	0.0007
659	1	62	4	58	0	61	4	57	3581.7987	3581.79862	0.0001
660	1	61	3	58	0	60	3	57	3581.8967	3581.89702	-0.0003
661	1	61	2	60	0	60	2	59	3581.9191	3581.91853	0.0006
662	1	60	1	59	0	59	1	58	3581.9288	3581.92951	-0.0007
663	1	60	2	58	0	59	2	57	3581.9611	3581.96093	0.0002
664	1	62	1	62	0	61	1	61	3582.0978	3582.09719	0.0006
665	1	63	4	60	0	62	4	59	3582.1474	3582.14796	-0.0006
666	1	62	3	60	0	61	3	59	3582.1492	3582.14877	0.0004
667	1	63	4	59	0	62	4	58	3582.1573	3582.15773	-0.0004
668	1	62	3	59	0	61	3	58	3582.2602	3582.26033	-0.0001
669	1	62	2	61	0	61	2	60	3582.2666	3582.26673	-0.0001
670	1	61	1	60	0	60	1	59	3582.2756	3582.27593	-0.0003
671	1	61	2	59	0	60	2	58	3582.3226	3582.32212	0.0005
672	1	63	1	63	0	62	1	62	3582.4404	3582.44009	0.0003
673	1	64	4	61	0	63	4	60	3582.5071	3582.50771	-0.0006
674	1	64	4	60	0	63	4	59	3582.5192	3582.51866	0.0005
675	1	63	2	62	0	62	2	61	3582.6164	3582.61637	0
676	1	62	1	61	0	61	1	60	3582.6233	3582.62347	-0.0002
677	1	63	3	60	0	62	3	59	3582.6258	3582.6257	0.0001
678	1	62	2	60	0	61	2	59	3582.6846	3582.68479	-0.0002
679	1	64	1	64	0	63	1	63	3582.7835	3582.78444	-0.0009
680	1	65	4	62	0	64	4	61	3582.8687	3582.86916	-0.0005
681	1	65	4	61	0	64	4	60	3582.8818	3582.88142	0.0004
682	1	64	2	63	0	63	2	62	3582.9679	3582.96744	0.0005
683	1	63	1	62	0	62	1	61	3582.972	3582.97211	-0.0001
684	1	64	3	61	0	63	3	60	3582.9925	3582.99313	-0.0006
685	1	63	2	61	0	62	2	60	3583.0483	3583.04892	-0.0006
686	1	65	1	65	0	64	1	64	3583.1306	3583.13025	0.0003
687	1	66	4	63	0	65	4	62	3583.2329	3583.2323	0.0006
688	1	66	4	62	0	65	4	61	3583.2454	3583.24599	-0.0006
689	1	65	2	64	0	64	2	63	3583.3198	3583.31992	-0.0001
690	1	64	1	63	0	63	1	62	3583.321	3583.32184	-0.0008
691	1	65	3	62	0	64	3	61	3583.3634	3583.36263	0.0008
692	1	64	2	62	0	63	2	61	3583.4148	3583.41449	0.0003
693	1	66	1	66	0	65	1	65	3583.4777	3583.47752	0.0002
694	1	67	4	64	0	66	4	63	3583.5967	3583.59713	-0.0004
695	1	67	4	63	0	66	4	62	3583.6127	3583.61239	0.0003
696	1	65	1	64	0	64	1	63	3583.6719	3583.67264	-0.0007
697	1	66	2	65	0	65	2	64	3583.6748	3583.6738	0.001
698	1	66	3	63	0	65	3	62	3583.7348	3583.73416	0.0006

699	1	65	2	63	0	64	2	62	3583.7821	3583.78146	0.0006
700	1	67	1	67	0	66	1	66	3583.8269	3583.82624	0.0007
701	1	68	4	65	0	67	4	64	3583.9638	3583.96364	0.0002
702	1	68	4	64	0	67	4	63	3583.9805	3583.98062	-0.0001
703	1	66	1	65	0	65	1	64	3584.0242	3584.02451	-0.0003
704	1	67	2	66	0	66	2	65	3584.0288	3584.02909	-0.0003
705	1	67	3	64	0	66	3	63	3584.1088	3584.10774	0.0011
706	1	66	2	64	0	65	2	63	3584.1505	3584.14983	0.0007
707	1	68	1	68	0	67	1	67	3584.1762	3584.1764	-0.0002
708	1	69	4	66	0	68	4	65	3584.3317	3584.33182	-0.0001
709	1	69	4	65	0	68	4	64	3584.3507	3584.35069	0
710	1	68	2	67	0	67	2	66	3584.3867	3584.38577	0.0009
711	1	67	2	65	0	66	2	64	3584.5202	3584.51956	0.0006
712	1	69	1	69	0	68	1	68	3584.528	3584.52801	0
713	1	70	4	67	0	69	4	66	3584.7024	3584.70166	0.0007
714	1	70	4	66	0	69	4	65	3584.7217	3584.72258	-0.0009
715	1	68	1	67	0	67	1	66	3584.7311	3584.73143	-0.0003
716	1	70	1	70	0	69	1	69	3584.8802	3584.88106	-0.0009
717	1	68	2	66	0	67	2	65	3584.8911	3584.89064	0.0005
718	1	69	1	68	0	68	1	67	3585.0863	3585.08647	-0.0002
719	1	69	2	67	0	68	2	66	3585.2628	3585.26304	-0.0002

B.4  $^{79}\text{BrNO } 3\nu_1$

N	v'	J'	K'_a	K'_c	v'	J''	K''_a	K''_c	Obs	Pred	Diff
1	1	63	8	55	0	64	8	56	5280.7741	5280.77426	-0.0002
2	1	62	8	54	0	63	8	55	5280.8366	5280.8376	-0.001
3	1	61	8	53	0	62	8	54	5280.9039	5280.9038	0.0001
4	1	60	8	52	0	61	8	53	5280.9738	5280.97287	0.0009
5	1	59	8	51	0	60	8	52	5281.0436	5281.04481	-0.0012
6	1	58	8	50	0	59	8	51	5281.1189	5281.11961	-0.0007
7	1	57	8	49	0	58	8	50	5281.1979	5281.19729	0.0006
8	1	56	8	48	0	57	8	49	5281.2792	5281.27784	0.0014
9	1	55	8	47	0	56	8	48	5281.3604	5281.36126	-0.0009
10	1	54	8	46	0	55	8	47	5281.4461	5281.44756	-0.0015
11	1	53	8	45	0	54	8	46	5281.5365	5281.53673	-0.0002
12	1	52	8	44	0	53	8	45	5281.6295	5281.62879	0.0007
13	1	51	8	43	0	52	8	44	5281.7247	5281.72372	0.001
14	1	50	8	42	0	51	8	43	5281.8206	5281.82154	-0.0009
15	1	49	8	41	0	50	8	42	5281.9207	5281.92224	-0.0015
16	1	63	7	56	0	64	7	57	5281.9542	5281.95451	-0.0003
17	1	62	7	55	0	63	7	56	5282.0184	5282.01767	0.0007
18	1	48	8	40	0	49	8	41	5282.0256	5282.02582	-0.0002
19	1	61	7	54	0	62	7	55	5282.0822	5282.08371	-0.0015

20	1	47	8	39	0	48	8	40	5282.1327	5282.13228	0.0004
21	1	60	7	53	0	61	7	54	5282.1536	5282.15261	0.001
22	1	59	7	52	0	60	7	53	5282.2253	5282.22439	0.0009
23	1	46	8	38	0	47	8	39	5282.2431	5282.24163	0.0015
24	1	58	7	51	0	59	7	52	5282.3003	5282.29904	0.0013
25	1	45	8	37	0	46	8	38	5282.3542	5282.35387	0.0003
26	1	57	7	50	0	58	7	51	5282.375	5282.37657	-0.0016
27	1	56	7	49	0	57	7	50	5282.4582	5282.45698	0.0012
28	1	44	8	36	0	45	8	37	5282.4673	5282.46899	-0.0017
29	1	55	7	48	0	56	7	49	5282.5413	5282.54027	0.001
30	1	43	8	35	0	44	8	36	5282.588	5282.587	0.001
31	1	54	7	47	0	55	7	48	5282.6279	5282.62644	0.0015
32	1	42	8	34	0	43	8	35	5282.7065	5282.70791	-0.0014
33	1	53	7	46	0	54	7	47	5282.7171	5282.71549	0.0016
34	1	52	7	45	0	53	7	46	5282.8082	5282.80742	0.0008
35	1	41	8	33	0	42	8	34	5282.8324	5282.83169	0.0007
36	1	49	7	42	0	50	7	43	5283.1009	5283.10054	0.0004
37	1	61	6	55	0	62	6	56	5283.1114	5283.11091	0.0005
38	1	48	7	41	0	49	7	42	5283.2047	5283.20402	0.0007
39	1	47	7	40	0	48	7	41	5283.31	5283.31038	-0.0004
40	1	58	6	52	0	59	6	53	5283.3263	5283.32561	0.0007
41	1	57	6	51	0	58	6	52	5283.4021	5283.40294	-0.0008
42	1	56	6	50	0	57	6	51	5283.4817	5283.48317	-0.0015
43	1	55	6	49	0	56	6	50	5283.5663	5283.56628	0
44	1	54	6	48	0	55	6	49	5283.6508	5283.65228	-0.0015
45	1	53	6	47	0	54	6	48	5283.7417	5283.74117	0.0005
46	1	52	6	46	0	53	6	47	5283.8316	5283.83296	-0.0014
47	1	51	6	45	0	52	6	46	5283.9265	5283.92763	-0.0011
48	1	60	5	55	0	61	5	56	5284.0522	5284.05304	-0.0008
49	1	59	5	54	0	60	5	55	5284.1249	5284.12426	0.0006
50	1	58	5	53	0	59	5	54	5284.1989	5284.1984	0.0005
51	1	69	4	66	0	70	4	67	5284.2647	5284.26384	0.0009
52	1	57	5	52	0	58	5	53	5284.2739	5284.27543	-0.0015
53	1	69	4	65	0	70	4	66	5284.2754	5284.27616	-0.0008
54	1	68	4	65	0	69	4	66	5284.3088	5284.30868	0.0001
55	1	68	4	64	0	69	4	65	5284.3196	5284.3196	0
56	1	56	5	51	0	57	5	52	5284.3545	5284.35537	-0.0009
57	1	67	4	64	0	68	4	65	5284.3553	5284.35639	-0.0011
58	1	67	4	63	0	68	4	64	5284.3653	5284.36607	-0.0008
59	1	66	4	63	0	67	4	64	5284.4082	5284.40699	0.0012
60	1	66	4	62	0	67	4	63	5284.4144	5284.41554	-0.0011
61	1	66	4	62	0	67	4	63	5284.4161	5284.41554	0.0006
62	1	55	5	50	0	56	5	51	5284.4388	5284.43822	0.0006
63	1	65	4	62	0	66	4	63	5284.4596	5284.46049	-0.0009
64	1	65	4	61	0	66	4	62	5284.4695	5284.46801	0.0015

65	1	64	4	61	0	65	4	62	5284.5181	5284.51687	0.0012
66	1	64	4	60	0	65	4	61	5284.5223	5284.52349	-0.0012
67	1	54	5	49	0	55	5	50	5284.5256	5284.52396	0.0016
68	1	63	4	59	0	64	4	60	5284.5833	5284.58195	0.0014
69	1	53	5	48	0	54	5	49	5284.6124	5284.61262	-0.0002
70	1	62	4	59	0	63	4	60	5284.6367	5284.63833	-0.0016
71	1	62	4	58	0	63	4	59	5284.6441	5284.6434	0.0007
72	1	50	5	45	0	51	5	46	5284.8961	5284.89601	0.0001
73	1	58	4	54	0	59	4	55	5284.9183	5284.91896	-0.0007
74	1	57	4	54	0	58	4	55	5284.9931	5284.9928	0.0003
75	1	57	4	53	0	58	4	54	5284.997	5284.99527	0.0017
76	1	49	5	44	0	50	5	45	5284.9974	5284.99629	0.0011
77	1	66	3	63	0	67	3	64	5285.0338	5285.03385	-0.0001
78	1	56	4	53	0	57	4	54	5285.0722	5285.07242	-0.0002
79	1	56	4	52	0	57	4	53	5285.0747	5285.07454	0.0002
80	1	65	3	62	0	66	3	63	5285.0828	5285.08171	0.0011
81	1	48	5	43	0	49	5	44	5285.1005	5285.09947	0.001
82	1	64	3	61	0	65	3	62	5285.1315	5285.13277	-0.0013
83	1	55	4	51	0	56	4	52	5285.1565	5285.15677	-0.0003
84	1	63	3	60	0	64	3	61	5285.1874	5285.18702	0.0004
85	1	47	5	42	0	48	5	43	5285.2051	5285.20556	-0.0005
86	1	67	2	66	0	68	2	67	5285.2131	5285.21317	-0.0001
87	1	69	1	69	0	70	1	70	5285.2358	5285.23505	0.0008
88	1	54	4	51	0	55	4	52	5285.2394	5285.2404	-0.001
89	1	54	4	50	0	55	4	51	5285.2405	5285.24195	-0.0014
90	1	61	3	59	0	62	3	60	5285.2548	5285.25324	0.0016
91	1	69	0	69	0	70	0	70	5285.2645	5285.2647	-0.0002
92	1	66	2	65	0	67	2	66	5285.2686	5285.27014	-0.0015
93	1	68	1	68	0	69	1	69	5285.2925	5285.29172	0.0008
94	1	61	3	58	0	62	3	59	5285.3059	5285.30511	0.0008
95	1	46	5	41	0	47	5	42	5285.3133	5285.31455	-0.0012
96	1	68	0	68	0	69	0	69	5285.3222	5285.32259	-0.0004
97	1	60	3	58	0	61	3	59	5285.3226	5285.3221	0.0005
98	1	53	4	50	0	54	4	51	5285.3273	5285.32877	-0.0015
99	1	53	4	49	0	54	4	50	5285.3301	5285.33008	0
100	1	67	1	67	0	68	1	68	5285.3502	5285.35097	-0.0008
101	1	69	1	68	0	70	1	69	5285.3583	5285.35829	0
102	1	60	3	57	0	61	3	58	5285.3684	5285.36893	-0.0005
103	1	68	2	66	0	69	2	67	5285.3796	5285.37862	0.001
104	1	67	0	67	0	68	0	68	5285.3836	5285.38307	0.0005
105	1	64	2	63	0	65	2	64	5285.3904	5285.39193	-0.0015
106	1	59	3	57	0	60	3	58	5285.3956	5285.39378	0.0018
107	1	66	1	66	0	67	1	67	5285.4111	5285.41279	-0.0017
108	1	68	1	67	0	69	1	68	5285.4125	5285.41166	0.0008
109	1	52	4	49	0	53	4	50	5285.4217	5285.42005	0.0017

110	1	52	4	48	0	53	4	49	5285.4221	5285.42115	0.0009
111	1	67	2	65	0	68	2	66	5285.4249	5285.42313	0.0018
112	1	59	3	56	0	60	3	57	5285.4358	5285.43594	-0.0001
113	1	66	0	66	0	67	0	67	5285.4451	5285.44615	-0.0011
114	1	63	2	62	0	64	2	63	5285.4577	5285.45676	0.0009
115	1	58	3	56	0	59	3	57	5285.4675	5285.46828	-0.0008
116	1	66	2	64	0	67	2	65	5285.4707	5285.47035	0.0003
117	1	65	1	65	0	66	1	66	5285.4758	5285.47719	-0.0014
118	1	65	0	65	0	66	0	66	5285.5116	5285.51183	-0.0002
119	1	51	4	47	0	52	4	48	5285.5161	5285.51517	0.0009
120	1	65	2	63	0	66	2	64	5285.5192	5285.52031	-0.0011
121	1	62	2	61	0	63	2	62	5285.5233	5285.52423	-0.0009
122	1	64	2	62	0	65	2	63	5285.5738	5285.57301	0.0008
123	1	64	0	64	0	65	0	65	5285.5814	5285.5801	0.0013
124	1	65	1	64	0	66	1	65	5285.5862	5285.58593	0.0003
125	1	61	2	60	0	62	2	61	5285.5936	5285.59434	-0.0007
126	1	50	4	46	0	51	4	47	5285.6115	5285.61213	-0.0006
127	1	50	4	47	0	51	4	48	5285.6126	5285.61135	0.0012
128	1	63	1	63	0	64	1	64	5285.6152	5285.61375	0.0015
129	1	63	2	61	0	64	2	62	5285.6295	5285.62849	0.001
130	1	64	1	63	0	65	1	64	5285.6482	5285.64878	-0.0006
131	1	63	0	63	0	64	0	64	5285.6506	5285.65097	-0.0004
132	1	56	3	53	0	57	3	54	5285.657	5285.65596	0.001
133	1	62	1	62	0	63	1	63	5285.6849	5285.68591	-0.001
134	1	62	2	60	0	63	2	61	5285.6867	5285.68675	0
135	1	36	6	30	0	37	6	31	5285.6954	5285.69513	0.0003
136	1	55	3	53	0	56	3	54	5285.7082	5285.70878	-0.0006
137	1	63	1	62	0	64	1	63	5285.7131	5285.71404	-0.0009
138	1	62	0	62	0	63	0	63	5285.7256	5285.72444	0.0012
139	1	55	3	52	0	56	3	53	5285.7346	5285.73561	-0.001
140	1	59	2	58	0	60	2	59	5285.7415	5285.74251	-0.001
141	1	61	2	59	0	62	2	60	5285.7477	5285.74782	-0.0001
142	1	61	1	61	0	62	1	62	5285.7622	5285.76066	0.0015
143	1	42	5	37	0	43	5	38	5285.7809	5285.77956	0.0013
144	1	62	1	61	0	63	1	62	5285.7818	5285.78171	0.0001
145	1	54	3	52	0	55	3	53	5285.7942	5285.79464	-0.0004
146	1	61	0	61	0	62	0	62	5285.8017	5285.8005	0.0012
147	1	60	2	58	0	61	2	59	5285.8105	5285.81172	-0.0012
148	1	48	4	44	0	49	4	45	5285.8149	5285.81487	0
149	1	54	3	51	0	55	3	52	5285.8172	5285.8184	-0.0012
150	1	58	2	57	0	59	2	58	5285.8209	5285.82059	0.0003
151	1	61	1	60	0	62	1	61	5285.851	5285.85182	-0.0008
152	1	59	2	57	0	60	2	58	5285.8771	5285.87847	-0.0014
153	1	60	0	60	0	61	0	61	5285.8796	5285.87916	0.0004
154	1	53	3	51	0	54	3	52	5285.8825	5285.88336	-0.0009

155	1	57	2	56	0	58	2	57	5285.902	5285.90135	0.0007
156	1	41	5	36	0	42	5	37	5285.9046	5285.90307	0.0015
157	1	53	3	50	0	54	3	51	5285.9057	5285.90431	0.0014
158	1	59	1	59	0	60	1	60	5285.9189	5285.91794	0.001
159	1	47	4	43	0	48	4	44	5285.9223	5285.92063	0.0017
160	1	60	1	59	0	61	1	60	5285.924	5285.92437	-0.0004
161	1	58	2	56	0	59	2	57	5285.9469	5285.94808	-0.0012
162	1	59	0	59	0	60	0	60	5285.9619	5285.9604	0.0015
163	1	52	3	50	0	53	3	51	5285.9763	5285.97494	0.0014
164	1	56	2	55	0	57	2	56	5285.9856	5285.98479	0.0008
165	1	52	3	49	0	53	3	50	5285.9949	5285.99335	0.0016
166	1	59	1	58	0	60	1	59	5285.9984	5285.9994	-0.001
167	1	58	1	58	0	59	1	59	5286.0006	5286.00048	0.0001
168	1	57	2	55	0	58	2	56	5286.0198	5286.02057	-0.0008
169	1	46	4	42	0	47	4	43	5286.0282	5286.02933	-0.0011
170	1	40	5	35	0	41	5	36	5286.0298	5286.02949	0.0003
171	1	58	0	58	0	59	0	59	5286.0457	5286.04424	0.0015
172	1	55	2	54	0	56	2	55	5286.0705	5286.07091	-0.0004
173	1	58	1	57	0	59	1	58	5286.0785	5286.07691	0.0016
174	1	51	3	48	0	52	3	49	5286.0862	5286.08549	0.0007
175	1	56	2	54	0	57	2	55	5286.0954	5286.09596	-0.0006
176	1	33	6	27	0	34	6	28	5286.1253	5286.12683	-0.0015
177	1	57	0	57	0	58	0	58	5286.1294	5286.13067	-0.0013
178	1	45	4	41	0	46	4	42	5286.1414	5286.14096	0.0004
179	1	57	1	56	0	58	1	57	5286.1574	5286.15692	0.0005
180	1	54	2	53	0	55	2	54	5286.1584	5286.15973	-0.0013
181	1	55	2	53	0	56	2	54	5286.1732	5286.17427	-0.0011
182	1	56	1	56	0	57	1	57	5286.1741	5286.17338	0.0007
183	1	50	3	47	0	51	3	48	5286.1822	5286.18073	0.0015
184	1	56	0	56	0	57	0	57	5286.2195	5286.21968	-0.0002
185	1	56	1	55	0	57	1	56	5286.2405	5286.23946	0.001
186	1	44	4	40	0	45	4	41	5286.2556	5286.25552	0.0001
187	1	55	1	55	0	56	1	56	5286.2621	5286.26374	-0.0016
188	1	49	3	47	0	50	3	48	5286.2658	5286.26689	-0.0011
189	1	32	6	26	0	33	6	27	5286.2751	5286.27652	-0.0014
190	1	49	3	46	0	50	3	47	5286.2779	5286.27906	-0.0012
191	1	38	5	33	0	39	5	34	5286.2904	5286.29103	-0.0006
192	1	55	0	55	0	56	0	56	5286.3108	5286.31128	-0.0005
193	1	55	1	54	0	56	1	55	5286.3262	5286.32454	0.0017
194	1	54	1	54	0	55	1	55	5286.3573	5286.35672	0.0006
195	1	48	3	46	0	49	3	47	5286.3692	5286.36996	-0.0008
196	1	43	4	39	0	44	4	40	5286.3743	5286.37301	0.0013
197	1	48	3	45	0	49	3	46	5286.3815	5286.38046	0.001
198	1	11	11	0	0	11	11	1	5286.4027	5286.40121	0.0015
199	1	54	0	54	0	55	0	55	5286.4041	5286.40546	-0.0014

200	1	54	1	53	0	55	1	54	5286.4132	5286.41219	0.001
201	1	37	5	32	0	38	5	33	5286.4276	5286.42616	0.0014
202	1	31	6	25	0	32	6	26	5286.4297	5286.42911	0.0006
203	1	12	11	1	0	12	11	2	5286.4361	5286.43545	0.0007
204	1	53	1	53	0	54	1	54	5286.4529	5286.45231	0.0006
205	1	47	3	45	0	48	3	46	5286.4768	5286.47592	0.0009
206	1	47	3	44	0	48	3	45	5286.486	5286.48493	0.0011
207	1	42	4	38	0	43	4	39	5286.4934	5286.49341	0
208	1	53	0	53	0	54	0	54	5286.5006	5286.50222	-0.0016
209	1	53	1	52	0	54	1	53	5286.5013	5286.50242	-0.0011
210	1	14	11	3	0	14	11	4	5286.5115	5286.51247	-0.001
211	1	52	1	52	0	53	1	53	5286.5498	5286.55053	-0.0007
212	1	15	11	4	0	15	11	5	5286.5567	5286.55526	0.0014
213	1	36	5	31	0	37	5	32	5286.5627	5286.56419	-0.0015
214	1	46	3	43	0	47	3	44	5286.5931	5286.59245	0.0007
215	1	16	11	5	0	16	11	6	5286.6013	5286.60089	0.0004
216	1	52	0	52	0	53	0	53	5286.6026	5286.60155	0.0011
217	1	17	11	6	0	17	11	7	5286.6494	5286.64937	0
218	1	51	1	51	0	52	1	52	5286.6507	5286.65136	-0.0007
219	1	45	3	43	0	46	3	44	5286.6972	5286.6965	0.0007
220	1	18	11	7	0	18	11	8	5286.7012	5286.70069	0.0005
221	1	45	3	42	0	46	3	43	5286.7021	5286.70302	-0.0009
222	1	35	5	30	0	36	5	31	5286.7062	5286.70512	0.0011
223	1	48	2	47	0	49	2	48	5286.75	5286.74973	0.0003
224	1	48	2	46	0	49	2	47	5286.8052	5286.8055	-0.0003
225	1	50	0	50	0	51	0	51	5286.8086	5286.80794	0.0007
226	1	44	3	42	0	45	3	43	5286.81	5286.81113	-0.0011
227	1	44	3	41	0	45	3	42	5286.8157	5286.81662	-0.0009
228	1	34	5	29	0	35	5	30	5286.8486	5286.84895	-0.0003
229	1	47	2	46	0	48	2	47	5286.8589	5286.85763	0.0013
230	1	39	4	35	0	40	4	36	5286.8716	5286.87216	-0.0006
231	1	47	2	45	0	48	2	46	5286.9063	5286.90772	-0.0014
232	1	49	0	49	0	50	0	50	5286.9159	5286.91498	0.0009
233	1	43	3	40	0	44	3	41	5286.9328	5286.93325	-0.0004
234	1	46	2	45	0	47	2	46	5286.9683	5286.9683	0
235	1	38	4	34	0	39	4	35	5287.0039	5287.00424	-0.0003
236	1	46	2	44	0	47	2	45	5287.0136	5287.01298	0.0006
237	1	48	0	48	0	49	0	49	5287.025	5287.0246	0.0004
238	1	42	3	40	0	43	3	41	5287.0506	5287.04909	0.0015
239	1	42	3	39	0	43	3	40	5287.0539	5287.05289	0.001
240	1	45	2	44	0	46	2	45	5287.0816	5287.08173	-0.0001
241	1	47	0	47	0	48	0	48	5287.138	5287.13678	0.0012
242	1	37	4	33	0	38	4	34	5287.1392	5287.13924	0
243	1	41	3	39	0	42	3	40	5287.1709	5287.17242	-0.0015
244	1	41	3	38	0	42	3	39	5287.1767	5287.17554	0.0012

245	1	46	0	46	0	47	0	47	5287.2508	5287.25153	-0.0007
246	1	36	4	32	0	37	4	33	5287.2785	5287.27716	0.0013
247	1	40	3	38	0	41	3	39	5287.2978	5287.29865	-0.0009
248	1	40	3	37	0	41	3	38	5287.301	5287.30119	-0.0002
249	1	45	1	45	0	46	1	46	5287.3123	5287.31169	0.0006
250	1	45	1	44	0	46	1	45	5287.3197	5287.31969	0
251	1	45	0	45	0	46	0	46	5287.3702	5287.36885	0.0014
252	1	35	4	31	0	36	4	32	5287.4173	5287.41798	-0.0007
253	1	39	3	37	0	40	3	38	5287.4294	5287.42779	0.0016
254	1	39	3	36	0	40	3	37	5287.4299	5287.42982	0.0001
255	1	44	1	44	0	45	1	45	5287.4314	5287.43101	0.0004
256	1	44	1	43	0	45	1	44	5287.4335	5287.43406	-0.0006
257	1	44	0	44	0	45	0	45	5287.4877	5287.48873	-0.001
258	1	43	1	42	0	44	1	43	5287.5507	5287.55121	-0.0005
259	1	43	1	43	0	44	1	44	5287.5543	5287.55297	0.0013
260	1	38	3	36	0	39	3	37	5287.561	5287.55984	0.0012
261	1	38	3	35	0	39	3	36	5287.5612	5287.56144	-0.0002
262	1	34	4	30	0	35	4	31	5287.5625	5287.56172	0.0008
263	1	42	1	41	0	43	1	42	5287.6698	5287.67115	-0.0013
264	1	42	1	42	0	43	1	43	5287.6757	5287.6776	-0.0019
265	1	37	3	35	0	38	3	36	5287.6959	5287.69479	0.0011
266	1	37	3	34	0	38	3	35	5287.6965	5287.69604	0.0005
267	1	41	1	40	0	42	1	41	5287.7936	5287.79389	-0.0003
268	1	41	1	41	0	42	1	42	5287.8049	5287.80489	0
269	1	39	2	38	0	40	2	39	5287.8194	5287.82068	-0.0013
270	1	39	2	37	0	40	2	38	5287.8368	5287.83591	0.0009
271	1	40	1	39	0	41	1	40	5287.9206	5287.91946	0.0011
272	1	40	1	40	0	41	1	41	5287.9337	5287.93484	-0.0011
273	1	38	2	37	0	39	2	38	5287.9538	5287.95362	0.0002
274	1	38	2	36	0	39	2	37	5287.9661	5287.96583	0.0003
275	1	39	1	39	0	40	1	40	5288.0678	5288.06747	0.0003
276	1	37	2	36	0	38	2	37	5288.0898	5288.08938	0.0004
277	1	13	10	4	0	13	10	3	5288.0951	5288.09556	-0.0005
278	1	37	2	35	0	38	2	36	5288.0987	5288.09885	-0.0001
279	1	14	10	4	0	14	10	5	5288.1343	5288.1355	-0.0012
280	1	14	10	5	0	14	10	4	5288.1345	5288.1355	-0.001
281	1	15	10	6	0	15	10	5	5288.1769	5288.17828	-0.0014
282	1	15	10	5	0	15	10	6	5288.1782	5288.17828	-0.0001
283	1	16	10	6	0	16	10	7	5288.2234	5288.22391	-0.0005
284	1	16	10	7	0	16	10	6	5288.2239	5288.22391	0
285	1	36	2	35	0	37	2	36	5288.2274	5288.22796	-0.0006
286	1	36	2	34	0	37	2	35	5288.2334	5288.23496	-0.0016
287	1	17	10	8	0	17	10	7	5288.273	5288.27239	0.0006
288	1	37	0	37	0	38	0	38	5288.4015	5288.39999	0.0015
289	1	21	10	12	0	21	10	11	5288.4938	5288.49473	-0.0009



290	1	21	10	11	0	21	10	12	5288.4962	5288.49473	0.0015
291	1	22	10	13	0	22	10	12	5288.5567	5288.55741	-0.0007
292	1	22	10	12	0	22	10	13	5288.5576	5288.55741	0.0002
293	1	35	0	35	0	36	0	36	5288.6832	5288.6837	-0.0005
294	1	34	1	33	0	35	1	34	5288.7316	5288.73289	-0.0013
295	1	34	0	34	0	35	0	35	5288.831	5288.82949	0.0015
296	1	33	1	32	0	34	1	33	5288.8772	5288.87858	-0.0014
297	1	33	0	33	0	34	0	34	5288.9789	5288.97791	0.001
298	1	32	1	31	0	33	1	32	5289.0289	5289.02719	0.0017
299	1	28	3	25	0	29	3	26	5289.0391	5289.04017	-0.0011
300	1	32	1	32	0	33	1	33	5289.0721	5289.07106	0.001
301	1	27	3	24	0	28	3	25	5289.2034	5289.20417	-0.0008
302	1	31	1	31	0	32	1	32	5289.2259	5289.22522	0.0007
303	1	26	3	23	0	27	3	24	5289.3714	5289.37109	0.0003
304	1	30	1	30	0	31	1	31	5289.3828	5289.38209	0.0007
305	1	28	2	26	0	29	2	27	5289.4351	5289.43454	0.0006
306	1	9	9	1	0	9	9	0	5289.4384	5289.44023	-0.0018
307	1	28	2	27	0	29	2	28	5289.4387	5289.4386	0.0001
308	1	10	9	2	0	10	9	1	5289.4699	5289.46877	0.0011
309	1	11	9	3	0	11	9	2	5289.5004	5289.50016	0.0002
310	1	12	9	4	0	12	9	3	5289.5335	5289.5344	-0.0009
311	1	25	3	22	0	26	3	23	5289.5414	5289.54091	0.0005
312	1	13	9	5	0	13	9	4	5289.5698	5289.57149	-0.0017
313	1	27	2	25	0	28	2	26	5289.5993	5289.59819	0.0011
314	1	27	2	26	0	28	2	27	5289.6033	5289.60275	0.0005
315	1	14	9	6	0	14	9	5	5289.612	5289.61143	0.0006
316	1	24	3	21	0	25	3	22	5289.7148	5289.71364	0.0012
317	1	26	2	24	0	27	2	25	5289.7666	5289.76486	0.0017
318	1	26	2	25	0	27	2	26	5289.7713	5289.76976	0.0015
319	1	23	3	20	0	24	3	21	5289.8903	5289.88928	0.001
320	1	25	2	24	0	26	2	25	5289.939	5289.93963	-0.0006
321	1	22	3	19	0	23	3	20	5290.0676	5290.06782	-0.0002
322	1	26	0	26	0	27	0	27	5290.0914	5290.09191	-0.0005
323	1	25	1	24	0	26	1	25	5290.1506	5290.14993	0.0007
324	1	21	3	18	0	22	3	19	5290.2492	5290.24925	-0.0001
325	1	25	0	25	0	26	0	26	5290.2617	5290.26195	-0.0002
326	1	24	1	23	0	25	1	24	5290.3237	5290.32219	0.0015
327	1	24	1	24	0	25	1	25	5290.38	5290.38046	-0.0005
328	1	20	3	17	0	21	3	18	5290.4326	5290.43358	-0.001
329	1	23	1	22	0	24	1	23	5290.4965	5290.49743	-0.0009
330	1	23	1	23	0	24	1	24	5290.5582	5290.55642	0.0018
331	1	19	3	16	0	20	3	17	5290.62	5290.6208	-0.0008
332	1	22	1	21	0	23	1	22	5290.6743	5290.67567	-0.0014
333	1	22	1	22	0	23	1	23	5290.734	5290.73511	-0.0011
334	1	8	8	0	0	8	8	1	5290.7429	5290.74114	0.0018

335	1	9	8	1	0	9	8	2	5290.7657	5290.76683	-0.0011
336	1	10	8	2	0	10	8	3	5290.795	5290.79536	-0.0004
337	1	18	3	15	0	19	3	16	5290.8119	5290.81091	0.001
338	1	11	8	3	0	11	8	4	5290.8265	5290.82675	-0.0003
339	1	12	8	4	0	12	8	5	5290.8612	5290.86099	0.0002
340	1	13	8	5	0	13	8	6	5290.8966	5290.89808	-0.0015
341	1	17	3	14	0	18	3	15	5291.0036	5291.00391	-0.0003
342	1	19	8	12	0	19	8	11	5291.1819	5291.1804	0.0015
343	1	16	3	13	0	17	3	14	5291.2004	5291.19979	0.0006
344	1	20	8	13	0	20	8	12	5291.2387	5291.23741	0.0013
345	1	21	8	14	0	21	8	13	5291.2981	5291.29727	0.0008
346	1	15	3	12	0	16	3	13	5291.3985	5291.39855	-0.0001
347	1	17	2	16	0	18	2	17	5291.4013	5291.40201	-0.0007
348	1	16	2	15	0	17	2	16	5291.597	5291.59776	-0.0008
349	1	15	2	14	0	16	2	15	5291.7975	5291.79639	0.0011
350	1	7	7	0	0	7	7	1	5291.8923	5291.89355	-0.0013
351	1	8	7	1	0	8	7	2	5291.9155	5291.91638	-0.0009
352	1	9	7	2	0	9	7	3	5291.9419	5291.94207	-0.0002
353	1	10	7	3	0	10	7	4	5291.9725	5291.97061	0.0019
354	1	14	2	13	0	15	2	14	5291.9968	5291.9979	-0.0011
355	1	11	7	4	0	11	7	5	5292.0035	5292.00199	0.0015
356	1	12	7	5	0	12	7	6	5292.0364	5292.03623	0.0002
357	1	14	7	7	0	14	7	8	5292.1119	5292.11326	-0.0014
358	1	15	7	8	0	15	7	9	5292.1569	5292.15605	0.0009
359	1	13	2	12	0	14	2	13	5292.201	5292.2023	-0.0013
360	1	16	7	9	0	16	7	10	5292.203	5292.20168	0.0013
361	1	14	1	13	0	15	1	14	5292.2106	5292.20952	0.0011
362	1	17	7	10	0	17	7	11	5292.2498	5292.25017	-0.0004
363	1	18	7	11	0	18	7	12	5292.3023	5292.30149	0.0008
364	1	19	7	12	0	19	7	13	5292.3551	5292.35566	-0.0006
365	1	13	1	12	0	14	1	13	5292.4145	5292.41479	-0.0003
366	1	12	1	11	0	13	1	12	5292.6241	5292.62306	0.001
367	1	11	1	10	0	12	1	11	5292.8359	5292.83435	0.0016
368	1	11	1	11	0	12	1	12	5292.8816	5292.88212	-0.0005
369	1	6	6	0	0	6	6	1	5292.8966	5292.8957	0.0009
370	1	7	6	1	0	7	6	2	5292.9143	5292.91568	-0.0014
371	1	8	6	2	0	8	6	3	5292.9372	5292.93851	-0.0013
372	1	9	6	3	0	9	6	4	5292.9656	5292.96419	0.0014
373	1	10	6	4	0	10	6	5	5292.9937	5292.99273	0.001
374	1	10	1	10	0	11	1	11	5293.0947	5293.09383	0.0009
375	1	9	1	9	0	10	1	10	5293.31	5293.30829	0.0017
376	1	5	5	0	0	5	5	1	5293.7469	5293.74604	0.0009
377	1	6	5	1	0	6	5	2	5293.7634	5293.76317	0.0002
378	1	7	5	2	0	7	5	3	5293.7827	5293.78315	-0.0005
379	1	8	5	3	0	8	5	4	5293.8047	5293.80598	-0.0013

380	1	20	5	15	0	20	5	16	5294.3027	5294.30241	0.0003
381	1	4	4	0	0	4	4	1	5294.4428	5294.44329	-0.0005
382	1	5	4	1	0	5	4	2	5294.4595	5294.45757	0.0019
383	1	6	4	2	0	6	4	3	5294.4765	5294.47469	0.0018
384	1	7	4	3	0	7	4	4	5294.4947	5294.49467	0
385	1	8	4	4	0	8	4	5	5294.5172	5294.51751	-0.0003
386	1	9	4	5	0	9	4	6	5294.5426	5294.5432	-0.0006
387	1	11	4	7	0	10	4	6	5297.2939	5297.29407	-0.0002
388	1	12	4	8	0	11	4	7	5297.5726	5297.57287	-0.0003
389	1	13	4	9	0	12	4	8	5297.8538	5297.8545	-0.0007
390	1	14	4	10	0	13	4	9	5298.1384	5298.13896	-0.0006
391	1	15	4	11	0	14	4	10	5298.4253	5298.42625	-0.001
392	1	14	3	11	0	13	3	10	5298.692	5298.69344	-0.0014
393	1	16	4	12	0	15	4	11	5298.7172	5298.71637	0.0008
394	1	15	3	12	0	14	3	11	5298.9805	5298.9808	-0.0003
395	1	17	4	13	0	16	4	12	5299.0106	5299.00932	0.0013
396	1	16	3	13	0	15	3	12	5299.2696	5299.27101	-0.0014
397	1	18	4	14	0	17	4	13	5299.3052	5299.30508	0.0001
398	1	15	2	14	0	14	2	13	5299.3752	5299.37516	0
399	1	14	0	14	0	13	0	13	5299.4006	5299.40114	-0.0005
400	1	21	5	16	0	20	5	15	5299.4998	5299.49796	0.0018
401	1	15	1	15	0	14	1	14	5299.5563	5299.5574	-0.0011
402	1	17	3	14	0	16	3	13	5299.5657	5299.56405	0.0016
403	1	19	4	15	0	18	4	14	5299.6041	5299.60367	0.0004
404	1	31	8	23	0	30	8	22	5299.6297	5299.63109	-0.0014
405	1	15	0	15	0	14	0	14	5299.6886	5299.68688	0.0017
406	1	22	5	17	0	21	5	16	5299.8042	5299.80494	-0.0007
407	1	16	1	16	0	15	1	15	5299.8426	5299.84228	0.0003
408	1	18	3	15	0	17	3	14	5299.8593	5299.85995	-0.0006
409	1	20	4	16	0	19	4	15	5299.9049	5299.90508	-0.0002
410	1	17	2	16	0	16	2	15	5299.9587	5299.95731	0.0014
411	1	32	8	24	0	31	8	23	5299.967	5299.96587	0.0011
412	1	16	0	16	0	15	0	15	5299.9745	5299.9752	-0.0007
413	1	23	5	18	0	22	5	17	5300.1137	5300.11473	-0.001
414	1	17	1	17	0	16	1	16	5300.1289	5300.12979	-0.0009
415	1	19	3	16	0	18	3	15	5300.1579	5300.15869	-0.0008
416	1	21	4	17	0	20	4	16	5300.2107	5300.2093	0.0014
417	1	18	2	17	0	17	2	16	5300.251	5300.25252	-0.0015
418	1	17	1	16	0	16	1	15	5300.2578	5300.25912	-0.0013
419	1	17	0	17	0	16	0	16	5300.2674	5300.26607	0.0013
420	1	33	8	25	0	32	8	24	5300.3035	5300.3034	0.0001
421	1	18	1	18	0	17	1	17	5300.4192	5300.41991	-0.0007
422	1	24	5	19	0	23	5	18	5300.4266	5300.42731	-0.0007
423	1	20	3	17	0	19	3	16	5300.4597	5300.46028	-0.0006
424	1	22	4	18	0	21	4	17	5300.5171	5300.51634	0.0008

425	1	19	2	18	0	18	2	17	5300.5517	5300.55048	0.0012
426	1	18	0	18	0	17	0	17	5300.5581	5300.55946	-0.0014
427	1	18	1	17	0	17	1	16	5300.5605	5300.55903	0.0015
428	1	34	8	26	0	33	8	25	5300.6427	5300.64367	-0.001
429	1	19	1	19	0	18	1	18	5300.711	5300.71264	-0.0016
430	1	25	5	20	0	24	5	19	5300.7423	5300.74269	-0.0004
431	1	21	3	18	0	20	3	17	5300.7658	5300.76471	0.0011
432	1	31	7	24	0	30	7	23	5300.8042	5300.80503	-0.0008
433	1	23	4	19	0	22	4	18	5300.8245	5300.82619	-0.0017
434	1	20	2	19	0	19	2	18	5300.8525	5300.85118	0.0013
435	1	19	0	19	0	18	0	18	5300.8556	5300.85535	0.0002
436	1	19	1	18	0	18	1	17	5300.8627	5300.86177	0.0009
437	1	35	8	27	0	34	8	26	5300.9856	5300.98669	-0.0011
438	1	20	1	20	0	19	1	19	5301.0064	5301.00796	-0.0016
439	1	26	5	21	0	25	5	20	5301.061	5301.06086	0.0001
440	1	22	3	19	0	21	3	18	5301.0733	5301.072	0.0013
441	1	24	4	20	0	23	4	19	5301.1381	5301.13885	-0.0008
442	1	32	7	25	0	31	7	24	5301.1393	5301.1398	-0.0005
443	1	20	0	20	0	19	0	19	5301.1536	5301.15372	-0.0001
444	1	21	2	20	0	20	2	19	5301.1547	5301.15461	0.0001
445	1	20	1	19	0	19	1	18	5301.1678	5301.16734	0.0005
446	1	21	1	21	0	20	1	20	5301.3058	5301.30587	-0.0001
447	1	36	8	28	0	35	8	27	5301.3313	5301.33245	-0.0012
448	1	27	5	22	0	26	5	21	5301.3821	5301.38183	0.0003
449	1	23	3	20	0	22	3	19	5301.3829	5301.38214	0.0008
450	1	22	2	21	0	21	2	20	5301.4597	5301.46076	-0.0011
451	1	33	7	26	0	32	7	25	5301.4768	5301.47732	-0.0005
452	1	21	1	20	0	20	1	19	5301.477	5301.47572	0.0013
453	1	22	1	22	0	21	1	21	5301.6054	5301.60637	-0.001
454	1	37	8	29	0	36	8	28	5301.6825	5301.68095	0.0016
455	1	24	3	21	0	23	3	20	5301.694	5301.69513	-0.0011
456	1	28	5	23	0	27	5	22	5301.7051	5301.70558	-0.0005
457	1	22	0	22	0	21	0	21	5301.758	5301.75775	0.0003
458	1	23	2	22	0	22	2	21	5301.77	5301.76963	0.0004
459	1	22	1	21	0	21	1	20	5301.788	5301.78689	0.0011
460	1	23	2	21	0	22	2	20	5301.7964	5301.79788	-0.0015
461	1	34	7	27	0	33	7	26	5301.819	5301.8176	0.0014
462	1	23	1	23	0	22	1	22	5301.909	5301.90943	-0.0004
463	1	25	3	22	0	24	3	21	5302.01	5302.01098	-0.001
464	1	29	5	24	0	28	5	23	5302.0307	5302.03211	-0.0014
465	1	24	2	23	0	23	2	22	5302.0807	5302.0812	-0.0005
466	1	27	4	23	0	26	4	22	5302.0922	5302.09369	-0.0015
467	1	23	1	22	0	22	1	21	5302.1	5302.10085	-0.0009
468	1	24	2	22	0	23	2	21	5302.1135	5302.11376	-0.0003
469	1	32	6	26	0	31	6	25	5302.1612	5302.16107	0.0001

470	1	35	7	28	0	34	7	27	5302.1614	5302.16062	0.0008
471	1	24	1	24	0	23	1	23	5302.2148	5302.21506	-0.0003
472	1	26	3	23	0	25	3	22	5302.3289	5302.3297	-0.0008
473	1	30	5	25	0	29	5	24	5302.36	5302.36143	-0.0014
474	1	24	0	24	0	23	0	23	5302.3698	5302.37134	-0.0015
475	1	39	8	31	0	38	8	30	5302.3867	5302.38612	0.0006
476	1	25	2	24	0	24	2	23	5302.3949	5302.39547	-0.0006
477	1	24	1	23	0	23	1	22	5302.4172	5302.41759	-0.0004
478	1	25	2	23	0	24	2	22	5302.4332	5302.43277	0.0004
479	1	33	6	27	0	32	6	26	5302.4989	5302.49862	0.0003
480	1	36	7	29	0	35	7	28	5302.5061	5302.50638	-0.0003
481	1	25	1	25	0	24	1	24	5302.5223	5302.52323	-0.0009
482	1	27	3	24	0	26	3	23	5302.6504	5302.65127	-0.0009
483	1	31	5	26	0	30	5	25	5302.6939	5302.69352	0.0004
484	1	26	2	25	0	25	2	24	5302.7116	5302.71242	-0.0008
485	1	25	1	24	0	24	1	23	5302.7377	5302.73707	0.0006
486	1	29	4	25	0	28	4	24	5302.743	5302.74426	-0.0013
487	1	40	8	32	0	39	8	31	5302.7431	5302.74279	0.0003
488	1	26	2	24	0	25	2	23	5302.7539	5302.75492	-0.001
489	1	26	1	26	0	25	1	25	5302.8345	5302.83396	0.0005
490	1	34	6	28	0	33	6	27	5302.8387	5302.83893	-0.0002
491	1	37	7	30	0	36	7	29	5302.8535	5302.85489	-0.0014
492	1	28	3	25	0	27	3	24	5302.9773	5302.97571	0.0016
493	1	26	0	26	0	25	0	25	5302.9937	5302.9943	-0.0006
494	1	32	5	27	0	31	5	26	5303.0291	5303.02839	0.0007
495	1	27	2	26	0	26	2	25	5303.0333	5303.03205	0.0012
496	1	26	1	25	0	25	1	24	5303.0583	5303.05929	-0.001
497	1	30	4	26	0	29	4	25	5303.0726	5303.07375	-0.0011
498	1	27	2	25	0	26	2	24	5303.0804	5303.08022	0.0002
499	1	41	8	33	0	40	8	32	5303.1031	5303.10217	0.0009
500	1	27	1	27	0	26	1	26	5303.1478	5303.14721	0.0006
501	1	35	6	29	0	34	6	28	5303.183	5303.18199	0.001
502	1	38	7	31	0	37	7	30	5303.2067	5303.20613	0.0006
503	1	29	3	26	0	28	3	25	5303.3037	5303.30302	0.0007
504	1	27	0	27	0	26	0	26	5303.3089	5303.30923	-0.0003
505	1	28	2	27	0	27	2	26	5303.3546	5303.35435	0.0003
506	1	33	5	28	0	32	5	27	5303.367	5303.36603	0.001
507	1	27	1	26	0	26	1	25	5303.3852	5303.38424	0.001
508	1	31	4	27	0	30	4	26	5303.4044	5303.40603	-0.0016
509	1	28	2	26	0	27	2	25	5303.4076	5303.40867	-0.0011
510	1	42	8	34	0	41	8	33	5303.463	5303.46427	-0.0013
511	1	28	1	28	0	27	1	27	5303.4633	5303.463	0.0003
512	1	36	6	30	0	35	6	29	5303.5275	5303.52781	-0.0003
513	1	28	0	28	0	27	0	27	5303.6276	5303.62643	0.0012
514	1	30	3	27	0	29	3	26	5303.6323	5303.63321	-0.0009

515	1	29	2	28	0	28	2	27	5303.6783	5303.6793	-0.001
516	1	34	5	29	0	33	5	28	5303.7078	5303.70644	0.0014
517	1	28	1	27	0	27	1	26	5303.7125	5303.71189	0.0006
518	1	29	2	27	0	28	2	26	5303.7406	5303.74029	0.0003
519	1	32	4	28	0	31	4	27	5303.7425	5303.74111	0.0014
520	1	29	1	29	0	28	1	28	5303.7821	5303.78129	0.0008
521	1	43	8	35	0	42	8	34	5303.8272	5303.82907	-0.0019
522	1	37	6	31	0	36	6	30	5303.8767	5303.87637	0.0003
523	1	40	7	33	0	39	7	32	5303.9179	5303.91679	0.0011
524	1	29	0	29	0	28	0	28	5303.9466	5303.94588	0.0007
525	1	31	3	28	0	30	3	27	5303.9677	5303.96628	0.0014
526	1	30	2	29	0	29	2	28	5304.006	5304.00689	-0.0009
527	1	29	1	28	0	28	1	27	5304.0431	5304.04222	0.0009
528	1	35	5	30	0	34	5	29	5304.0505	5304.04962	0.0009
529	1	30	2	28	0	29	2	27	5304.0743	5304.07507	-0.0008
530	1	33	4	29	0	32	4	28	5304.0784	5304.07898	-0.0006
531	1	30	1	30	0	29	1	29	5304.1025	5304.1021	0.0004
532	1	30	0	30	0	29	0	29	5304.2676	5304.26756	0
533	1	32	3	29	0	31	3	28	5304.3005	5304.30223	-0.0017
534	1	31	2	30	0	30	2	29	5304.3372	5304.33713	0.0001
535	1	30	1	29	0	29	1	28	5304.3739	5304.37523	-0.0013
536	1	36	5	31	0	35	5	30	5304.3965	5304.39556	0.0009
537	1	31	2	29	0	30	2	28	5304.4116	5304.41301	-0.0014
538	1	31	1	31	0	30	1	30	5304.424	5304.42541	-0.0014
539	1	31	0	31	0	30	0	30	5304.5902	5304.59146	-0.0013
540	1	33	3	30	0	32	3	29	5304.6411	5304.64107	0
541	1	32	2	31	0	31	2	30	5304.6689	5304.66998	-0.0011
542	1	31	1	30	0	30	1	29	5304.7122	5304.71089	0.0013
543	1	32	1	32	0	31	1	31	5304.7504	5304.7512	-0.0008
544	1	32	2	30	0	31	2	29	5304.7554	5304.75412	0.0013
545	1	32	0	32	0	31	0	31	5304.9165	5304.91755	-0.0011
546	1	34	3	32	0	33	3	31	5304.977	5304.97658	0.0004
547	1	34	3	31	0	33	3	30	5304.9841	5304.98281	0.0013
548	1	33	2	32	0	32	2	31	5305.0045	5305.00545	-0.001
549	1	32	1	31	0	31	1	30	5305.05	5305.04917	0.0008
550	1	33	1	33	0	32	1	32	5305.0808	5305.07947	0.0013
551	1	38	5	33	0	37	5	32	5305.0959	5305.0957	0.0002
552	1	33	2	31	0	32	2	30	5305.099	5305.09839	0.0006
553	1	33	0	33	0	32	0	32	5305.2452	5305.24584	-0.0006
554	1	35	3	33	0	34	3	32	5305.3216	5305.32016	0.0014
555	1	35	3	32	0	34	3	31	5305.3276	5305.32746	0.0001
556	1	34	2	33	0	33	2	32	5305.343	5305.34353	-0.0005
557	1	33	1	32	0	32	1	31	5305.3919	5305.39007	0.0018
558	1	34	1	34	0	33	1	33	5305.4109	5305.41022	0.0007
559	1	34	2	32	0	33	2	31	5305.4446	5305.44582	-0.0012

560	1	39	5	34	0	38	5	33	5305.4499	5305.4499	0
561	1	37	4	33	0	36	4	32	5305.4591	5305.45836	0.0007
562	1	34	0	34	0	33	0	33	5305.575	5305.5763	-0.0013
563	1	36	3	34	0	35	3	33	5305.666	5305.66651	-0.0005
564	1	36	3	33	0	35	3	32	5305.6744	5305.67502	-0.0006
565	1	35	2	34	0	34	2	33	5305.6837	5305.68419	-0.0005
566	1	34	1	33	0	33	1	32	5305.7344	5305.73355	0.0008
567	1	35	2	33	0	34	2	32	5305.7966	5305.79639	0.0002
568	1	40	5	35	0	39	5	34	5305.8061	5305.80685	-0.0008
569	1	38	4	34	0	37	4	33	5305.8097	5305.81017	-0.0005
570	1	35	0	35	0	34	0	34	5305.9079	5305.90893	-0.001
571	1	37	3	35	0	36	3	34	5306.017	5306.01562	0.0014
572	1	36	2	35	0	35	2	34	5306.0259	5306.02743	-0.0015
573	1	37	3	34	0	36	3	33	5306.0268	5306.02549	0.0013
574	1	35	1	34	0	34	1	33	5306.0801	5306.0796	0.0005
575	1	36	2	34	0	35	2	33	5306.1506	5306.15009	0.0005
576	1	39	4	35	0	38	4	34	5306.1631	5306.16476	-0.0017
577	1	36	0	36	0	35	0	35	5306.2432	5306.24373	-0.0005
578	1	38	3	36	0	37	3	35	5306.3687	5306.36748	0.0012
579	1	37	2	36	0	36	2	35	5306.3743	5306.37325	0.0011
580	1	38	3	35	0	37	3	34	5306.3801	5306.3789	0.0012
581	1	37	1	37	0	36	1	36	5306.4186	5306.4172	0.0014
582	1	36	1	35	0	35	1	34	5306.4286	5306.42819	0.0004
583	1	37	2	35	0	36	2	34	5306.5065	5306.50691	-0.0004
584	1	40	4	36	0	39	4	35	5306.5237	5306.52213	0.0016
585	1	37	0	37	0	36	0	36	5306.5803	5306.58068	-0.0004
586	1	38	2	37	0	37	2	36	5306.7199	5306.72162	-0.0017
587	1	39	3	37	0	38	3	36	5306.7219	5306.72209	-0.0002
588	1	39	3	36	0	38	3	35	5306.7364	5306.73524	0.0012
589	1	37	1	36	0	36	1	35	5306.7808	5306.7793	0.0015
590	1	38	2	36	0	37	2	35	5306.8687	5306.86684	0.0019
591	1	41	4	37	0	40	4	36	5306.8811	5306.88229	-0.0012
592	1	38	0	38	0	37	0	37	5306.9196	5306.9198	-0.0002
593	1	39	2	38	0	38	2	37	5307.0726	5307.07253	0.0001
594	1	40	3	38	0	39	3	37	5307.079	5307.07943	-0.0004
595	1	40	3	37	0	39	3	36	5307.0932	5307.09452	-0.0013
596	1	39	1	39	0	38	1	38	5307.1013	5307.10072	0.0006
597	1	38	1	37	0	37	1	36	5307.1313	5307.13291	-0.0016
598	1	39	2	37	0	38	2	36	5307.2292	5307.22984	-0.0006
599	1	42	4	38	0	41	4	37	5307.2446	5307.24522	-0.0006
600	1	39	0	39	0	38	0	38	5307.2598	5307.26107	-0.0013
601	1	40	2	39	0	39	2	38	5307.4244	5307.42598	-0.0016
602	1	41	3	39	0	40	3	38	5307.4384	5307.43951	-0.0011
603	1	40	1	40	0	39	1	39	5307.4466	5307.44612	0.0005
604	1	41	3	38	0	40	3	37	5307.4564	5307.45676	-0.0004

605	1	39	1	38	0	38	1	37	5307.4886	5307.48899	-0.0004
606	1	40	2	38	0	39	2	37	5307.5957	5307.59591	-0.0002
607	1	43	4	39	0	42	4	38	5307.6105	5307.61093	-0.0004
608	1	41	1	41	0	40	1	40	5307.7926	5307.79394	-0.0013
609	1	42	3	40	0	41	3	39	5307.8035	5307.80231	0.0012
610	1	42	3	39	0	41	3	38	5307.8232	5307.82197	0.0012
611	1	40	1	39	0	39	1	38	5307.847	5307.84751	-0.0005
612	1	41	0	41	0	40	0	40	5307.95	5307.95011	-0.0001
613	1	41	2	39	0	40	2	38	5307.9666	5307.96502	0.0016
614	1	44	4	40	0	43	4	39	5307.9795	5307.97941	0.0001
615	1	42	1	42	0	41	1	41	5308.1445	5308.14415	0.0003
616	1	43	3	41	0	42	3	40	5308.1677	5308.16782	-0.0001
617	1	43	3	40	0	42	3	39	5308.19	5308.19015	-0.0001
618	1	41	1	40	0	40	1	39	5308.2075	5308.20845	-0.0009
619	1	42	2	40	0	41	2	39	5308.3364	5308.33713	-0.0007
620	1	45	4	41	0	44	4	40	5308.3518	5308.35067	0.0011
621	1	43	1	43	0	42	1	42	5308.4976	5308.49677	0.0008
622	1	43	2	42	0	42	2	41	5308.5018	5308.5014	0.0004
623	1	44	3	42	0	43	3	41	5308.5355	5308.53603	-0.0005
624	1	44	3	41	0	43	3	40	5308.5606	5308.56132	-0.0007
625	1	42	1	41	0	41	1	40	5308.5701	5308.57178	-0.0017
626	1	43	0	43	0	42	0	42	5308.6464	5308.64785	-0.0014
627	1	43	2	41	0	42	2	40	5308.7128	5308.71223	0.0006
628	1	46	4	42	0	45	4	41	5308.7265	5308.7247	0.0018
629	1	44	1	44	0	43	1	43	5308.8509	5308.85178	-0.0009
630	1	44	2	43	0	43	2	42	5308.8643	5308.86487	-0.0006
631	1	45	3	43	0	44	3	42	5308.9057	5308.90694	-0.0012
632	1	45	3	42	0	44	3	41	5308.9372	5308.93548	0.0017
633	1	43	1	42	0	42	1	41	5308.9388	5308.93747	0.0013
634	1	44	0	44	0	43	0	43	5308.9992	5309	-0.0008
635	1	44	2	42	0	43	2	41	5309.0888	5309.09028	-0.0015
636	1	47	4	43	0	46	4	42	5309.1018	5309.10151	0.0003
637	1	45	1	45	0	44	1	44	5309.2091	5309.20917	-0.0001
638	1	45	2	44	0	44	2	43	5309.2303	5309.2308	-0.0005
639	1	46	3	44	0	45	3	43	5309.2789	5309.28054	-0.0016
640	1	44	1	43	0	43	1	42	5309.3049	5309.3055	-0.0006
641	1	46	3	43	0	45	3	42	5309.3138	5309.31266	0.0011
642	1	45	0	45	0	44	0	44	5309.3537	5309.35435	-0.0007
643	1	52	6	46	0	51	6	45	5309.4311	5309.43142	-0.0003
644	1	45	2	43	0	44	2	42	5309.472	5309.47125	0.0007
645	1	48	4	44	0	47	4	43	5309.4818	5309.48109	0.0007
646	1	46	1	46	0	45	1	45	5309.5686	5309.56894	-0.0003
647	1	46	2	45	0	45	2	44	5309.6004	5309.59919	0.0012
648	1	47	3	45	0	46	3	44	5309.6557	5309.6568	-0.0011
649	1	45	1	44	0	44	1	43	5309.675	5309.67583	-0.0008



650	1	47	3	44	0	46	3	43	5309.6926	5309.69285	-0.0002
651	1	46	0	46	0	45	0	45	5309.7104	5309.71092	-0.0005
652	1	53	6	47	0	52	6	46	5309.823	5309.82333	-0.0003
653	1	46	2	44	0	45	2	43	5309.854	5309.85511	-0.0011
654	1	49	4	45	0	48	4	44	5309.8621	5309.86344	-0.0013
655	1	47	1	47	0	46	1	46	5309.9319	5309.93108	0.0008
656	1	47	2	46	0	46	2	45	5309.9706	5309.97003	0.0006
657	1	48	3	46	0	47	3	45	5310.0343	5310.03573	-0.0014
658	1	46	1	45	0	45	1	44	5310.0471	5310.04843	-0.0013
659	1	48	3	45	0	47	3	44	5310.0766	5310.07608	0.0005
660	1	54	6	48	0	53	6	47	5310.2187	5310.21791	0.0008
661	1	47	2	45	0	46	2	44	5310.2421	5310.24183	0.0003
662	1	50	4	46	0	49	4	45	5310.2493	5310.24856	0.0007
663	1	48	1	48	0	47	1	47	5310.2954	5310.29559	-0.0002
664	1	49	3	47	0	48	3	46	5310.4173	5310.41731	0
665	1	47	1	46	0	46	1	45	5310.4249	5310.42328	0.0016
666	1	49	3	46	0	48	3	45	5310.4633	5310.46235	0.001
667	1	48	2	46	0	47	2	45	5310.6313	5310.63136	-0.0001
668	1	51	4	48	0	50	4	47	5310.6336	5310.63358	0
669	1	51	4	47	0	50	4	46	5310.6351	5310.63646	-0.0014
670	1	49	0	49	0	48	0	48	5310.7938	5310.79401	-0.0002
671	1	48	1	47	0	47	1	46	5310.8001	5310.80035	-0.0002
672	1	50	3	47	0	49	3	46	5310.852	5310.85167	0.0003
673	1	52	4	48	0	51	4	47	5311.0289	5311.02713	0.0018
674	1	53	4	50	0	52	4	49	5311.4181	5311.41673	0.0014
675	1	53	4	49	0	52	4	48	5311.4194	5311.42057	-0.0012
676	1	54	4	51	0	53	4	50	5311.812	5311.81237	-0.0004
677	1	55	4	52	0	54	4	51	5312.2095	5312.21071	-0.0012
678	1	55	4	51	0	54	4	50	5312.2151	5312.21577	-0.0007
679	1	56	4	53	0	55	4	52	5312.6106	5312.61175	-0.0012
680	1	56	4	52	0	55	4	51	5312.6162	5312.61754	-0.0013
681	1	57	4	54	0	56	4	53	5313.0159	5313.01548	0.0004
682	1	57	4	53	0	56	4	52	5313.0213	5313.02208	-0.0008
683	1	58	4	55	0	57	4	54	5313.4218	5313.42189	-0.0001
684	1	58	4	54	0	57	4	53	5313.4291	5313.4294	-0.0003
685	1	62	6	56	0	61	6	55	5313.4695	5313.47006	-0.0006

B.5  $^{81}\text{BrNO } 3\nu_1$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu''$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	11	11	0	0	11	11	1	5286.3714	5286.37111	0.0003
2	1	12	11	1	0	12	11	2	5286.4041	5286.4052	-0.0011
3	1	13	11	2	0	13	11	3	5286.4429	5286.44212	0.0008
4	1	14	11	3	0	14	11	4	5286.4826	5286.48188	0.0007

5	1	15	11	4	0	15	11	5	5286.524	5286.52448	-0.0005
6	1	16	11	5	0	16	11	6	5286.5699	5286.56991	0
7	1	17	11	6	0	17	11	7	5286.6179	5286.61817	-0.0003
8	1	18	11	7	0	18	11	8	5286.6682	5286.66927	-0.0011
9	1	19	11	8	0	19	11	9	5286.7222	5286.72319	-0.001
10	1	10	10	0	0	10	10	1	5287.9635	5287.96427	-0.0008
11	1	10	10	0	0	10	10	1	5287.965	5287.96427	0.0007
12	1	11	10	1	0	11	10	2	5287.9958	5287.99552	0.0003
13	1	11	10	1	0	11	10	2	5287.9955	5287.99552	0
14	1	12	10	2	0	12	10	3	5288.0289	5288.02961	-0.0007
15	1	12	10	2	0	12	10	3	5288.0308	5288.02961	0.0012
16	1	13	10	3	0	13	10	4	5288.0659	5288.06653	-0.0006
17	1	13	10	3	0	13	10	4	5288.0659	5288.06653	-0.0006
18	1	14	10	4	0	14	10	5	5288.1074	5288.10629	0.0011
19	1	14	10	4	0	14	10	5	5288.1073	5288.10629	0.001
20	1	15	10	5	0	15	10	6	5288.1478	5288.14888	-0.0011
21	1	15	10	5	0	15	10	6	5288.15	5288.14888	0.0011
22	1	16	10	6	0	16	10	7	5288.1955	5288.19431	0.0012
23	1	16	10	6	0	16	10	7	5288.1955	5288.19431	0.0012
24	1	17	10	7	0	17	10	8	5288.2435	5288.24257	0.0009
25	1	17	10	7	0	17	10	8	5288.2417	5288.24257	-0.0009
26	1	18	10	8	0	18	10	9	5288.2934	5288.29366	-0.0003
27	1	18	10	8	0	18	10	9	5288.2932	5288.29366	-0.0005
28	1	19	10	9	0	19	10	10	5288.348	5288.34759	0.0004
29	1	19	10	9	0	19	10	10	5288.3472	5288.34759	-0.0004
30	1	20	10	10	0	20	10	11	5288.405	5288.40434	0.0007
31	1	20	10	10	0	20	10	11	5288.4037	5288.40434	-0.0006
32	1	21	10	11	0	21	10	12	5288.4641	5288.46392	0.0002
33	1	21	10	11	0	21	10	12	5288.464	5288.46392	0.0001
34	1	22	10	12	0	22	10	13	5288.5251	5288.52632	-0.0012
35	1	22	10	12	0	22	10	13	5288.5268	5288.52632	0.0005
36	1	23	10	13	0	23	10	14	5288.5926	5288.59155	0.001
37	1	23	10	13	0	23	10	14	5288.5915	5288.59155	-0.0001
38	1	24	10	14	0	24	10	15	5288.6603	5288.65961	0.0007
39	1	24	10	14	0	24	10	15	5288.6599	5288.65961	0.0003
40	1	25	10	15	0	25	10	16	5288.7308	5288.73048	0.0003
41	1	25	10	15	0	25	10	16	5288.7306	5288.73048	0.0001
42	1	26	10	16	0	26	10	17	5288.8038	5288.80418	-0.0004
43	1	26	10	16	0	26	10	17	5288.8057	5288.80418	0.0015
44	1	27	10	17	0	27	10	18	5288.8807	5288.88069	0
45	1	28	10	18	0	28	10	19	5288.9595	5288.96002	-0.0005
46	1	9	9	0	0	9	9	1	5289.4116	5289.41282	-0.0012
47	1	10	9	1	0	10	9	2	5289.4405	5289.44122	-0.0007
48	1	11	9	2	0	11	9	3	5289.4718	5289.47247	-0.0007
49	1	12	9	3	0	12	9	4	5289.507	5289.50656	0.0004

50	1	13	9	4	0	13	9	5	5289.5438	5289.54348	0.0003
51	1	14	9	5	0	14	9	6	5289.5835	5289.58323	0.0003
52	1	15	9	6	0	15	9	7	5289.6246	5289.62583	-0.0012
53	1	16	9	7	0	16	9	8	5289.6721	5289.67125	0.0008
54	1	17	9	8	0	17	9	9	5289.7201	5289.71951	0.0006
55	1	18	9	9	0	18	9	10	5289.7712	5289.7706	0.0006
56	1	19	9	10	0	19	9	11	5289.8241	5289.82453	-0.0004
57	1	20	9	11	0	20	9	12	5289.8827	5289.88128	0.0014
58	1	21	9	12	0	21	9	13	5289.9395	5289.94086	-0.0014
59	1	22	9	13	0	22	9	14	5290.0031	5290.00326	-0.0002
60	1	23	9	14	0	23	9	15	5290.0677	5290.06849	-0.0008
61	1	24	9	15	0	24	9	16	5290.1355	5290.13655	-0.001
62	1	25	9	16	0	25	9	17	5290.2064	5290.20742	-0.001
63	1	26	9	17	0	26	9	18	5290.28	5290.28112	-0.0011
64	1	27	9	18	0	27	9	19	5290.3579	5290.35764	0.0003
65	1	8	8	0	0	8	8	1	5290.7136	5290.71457	-0.001
66	1	9	8	1	0	9	8	2	5290.7398	5290.74014	-0.0003
67	1	10	8	2	0	10	8	3	5290.7695	5290.76854	0.001
68	1	11	8	3	0	11	8	4	5290.8	5290.79979	0.0002
69	1	12	8	4	0	12	8	5	5290.8325	5290.83387	-0.0014
70	1	13	8	5	0	13	8	6	5290.87	5290.87079	-0.0008
71	1	14	8	6	0	14	8	7	5290.9109	5290.91055	0.0004
72	1	15	8	7	0	15	8	8	5290.9537	5290.95314	0.0006
73	1	16	8	8	0	16	8	9	5290.998	5290.99857	-0.0006
74	1	17	8	9	0	17	8	10	5291.0468	5291.04683	0
75	1	18	8	10	0	18	8	11	5291.0978	5291.09792	-0.0001
76	1	19	8	11	0	19	8	12	5291.1512	5291.15184	-0.0006
77	1	20	8	12	0	20	8	13	5291.2095	5291.20859	0.0009
78	1	21	8	13	0	21	8	14	5291.269	5291.26817	0.0008
79	1	22	8	14	0	22	8	15	5291.3307	5291.33058	0.0001
80	1	23	8	15	0	23	8	16	5291.3963	5291.39581	0.0005
81	1	24	8	16	0	24	8	17	5291.4637	5291.46387	-0.0002
82	1	25	8	17	0	25	8	18	5291.536	5291.53475	0.0012
83	1	26	8	18	0	26	8	19	5291.6082	5291.60846	-0.0003
84	1	7	7	0	0	7	7	1	5291.868	5291.86758	0.0004
85	1	8	7	1	0	8	7	2	5291.8908	5291.89031	0.0005
86	1	9	7	2	0	9	7	3	5291.915	5291.91588	-0.0009
87	1	10	7	3	0	10	7	4	5291.9449	5291.94429	0.0006
88	1	11	7	4	0	11	7	5	5291.9754	5291.97553	-0.0001
89	1	12	7	5	0	12	7	6	5292.0096	5292.00961	0
90	1	13	7	6	0	13	7	7	5292.0457	5292.04654	-0.0008
91	1	14	7	7	0	14	7	8	5292.0872	5292.08629	0.0009
92	1	15	7	8	0	15	7	9	5292.1278	5292.12888	-0.0011
93	1	16	7	9	0	16	7	10	5292.1736	5292.17431	-0.0007
94	1	17	7	10	0	17	7	11	5292.2228	5292.22257	0.0002

95	1	18	7	11	0	18	7	12	5292.2738	5292.27366	0.0001
96	1	19	7	12	0	19	7	13	5292.3282	5292.32759	0.0006
97	1	20	7	13	0	20	7	14	5292.3841	5292.38434	-0.0002
98	1	21	7	14	0	21	7	15	5292.4447	5292.44393	0.0008
99	1	22	7	15	0	22	7	16	5292.5073	5292.50634	0.001
100	1	23	7	16	0	23	7	17	5292.5706	5292.57158	-0.001
101	1	6	6	0	0	6	6	1	5292.869	5292.87015	-0.0011
102	1	7	6	1	0	7	6	2	5292.891	5292.89004	0.001
103	1	8	6	2	0	8	6	3	5292.9116	5292.91276	-0.0012
104	1	9	6	3	0	9	6	4	5292.9393	5292.93833	0.001
105	1	10	6	4	0	10	6	5	5292.9659	5292.96674	-0.0008
106	1	11	6	5	0	11	6	6	5292.9989	5292.99798	0.0009
107	1	12	6	6	0	12	6	7	5293.0316	5293.03207	-0.0005
108	1	13	6	7	0	13	6	8	5293.0692	5293.06899	0.0002
109	1	14	6	8	0	14	6	9	5293.1077	5293.10874	-0.001
110	1	15	6	9	0	15	6	10	5293.1516	5293.15134	0.0003
111	1	16	6	10	0	16	6	11	5293.196	5293.19677	-0.0008
112	1	17	6	11	0	17	6	12	5293.2449	5293.24503	-0.0001
113	1	18	6	12	0	18	6	13	5293.2949	5293.29613	-0.0012
114	1	19	6	13	0	19	6	14	5293.3511	5293.35006	0.001
115	1	20	6	14	0	20	6	15	5293.4074	5293.40683	0.0006
116	1	21	6	15	0	21	6	16	5293.4651	5293.46642	-0.0013
117	1	22	6	16	0	22	6	17	5293.5295	5293.52884	0.0007
118	1	5	5	0	0	5	5	1	5293.7218	5293.72077	0.001
119	1	6	5	1	0	6	5	2	5293.7388	5293.73782	0.001
120	1	7	5	2	0	7	5	3	5293.7586	5293.7577	0.0009
121	1	8	5	3	0	8	5	4	5293.7809	5293.78043	0.0005
122	1	9	5	4	0	9	5	5	5293.8059	5293.806	-0.0001
123	1	10	5	5	0	10	5	6	5293.8358	5293.83441	0.0014
124	1	11	5	6	0	11	5	7	5293.8664	5293.86565	0.0007
125	1	12	5	7	0	12	5	8	5293.8997	5293.89974	0
126	1	13	5	8	0	13	5	9	5293.9377	5293.93666	0.001
127	1	14	5	9	0	14	5	10	5293.977	5293.97643	0.0006
128	1	15	5	10	0	15	5	11	5294.019	5294.01903	0
129	1	16	5	11	0	16	5	12	5294.0649	5294.06446	0.0004
130	1	17	5	12	0	17	5	13	5294.112	5294.11274	-0.0007
131	1	18	5	13	0	18	5	14	5294.1647	5294.16385	0.0009
132	1	19	5	14	0	19	5	15	5294.2175	5294.21779	-0.0003
133	1	20	5	15	0	20	5	16	5294.2737	5294.27457	-0.0009
134	1	4	4	0	0	4	4	1	5294.4186	5294.41819	0.0004
135	1	5	4	1	0	5	4	2	5294.4317	5294.4324	-0.0007
136	1	6	4	2	0	6	4	3	5294.4484	5294.44944	-0.001
137	1	7	4	3	0	7	4	4	5294.4695	5294.46933	0.0002
138	1	8	4	4	0	8	4	5	5294.4933	5294.49206	0.0012
139	1	9	4	5	0	9	4	6	5294.5184	5294.51763	0.0008

140	1	10	4	6	0	10	4	7	5294.5454	5294.54604	-0.0006
141	1	11	4	7	0	11	4	8	5294.5785	5294.57729	0.0012
142	1	12	4	8	0	12	4	9	5294.6099	5294.61139	-0.0015
143	1	13	4	9	0	13	4	10	5294.6481	5294.64832	-0.0002
144	1	14	4	10	0	14	4	11	5294.6876	5294.68809	-0.0005
145	1	15	4	11	0	15	4	12	5294.7318	5294.7307	0.0011
146	1	16	4	12	0	16	4	13	5294.7763	5294.77616	0.0001
147	1	17	4	13	0	17	4	14	5294.825	5294.82445	0.0006
148	1	18	4	14	0	18	4	15	5294.8767	5294.87558	0.0011
149	1	19	4	15	0	19	4	16	5294.9292	5294.92955	-0.0004
150	1	20	4	16	0	20	4	17	5294.9852	5294.98636	-0.0012
151	1	6	5	1	0	5	5	0	5295.1962	5295.19645	-0.0003
152	1	7	5	2	0	6	5	1	5295.4589	5295.45942	-0.0005
153	1	8	5	3	0	7	5	2	5295.725	5295.72521	-0.0002
154	1	6	4	2	0	5	4	1	5295.9079	5295.90789	0
155	1	9	5	4	0	8	5	3	5295.9938	5295.99383	0
156	1	2	1	2	0	1	1	1	5296.067	5296.06815	-0.0012
157	1	2	1	1	0	1	1	0	5296.0786	5296.07951	-0.0009
158	1	3	2	1	0	2	2	0	5296.0872	5296.08721	0
159	1	7	4	3	0	6	4	2	5296.1696	5296.17082	-0.0012
160	1	5	3	2	0	4	3	1	5296.2026	5296.20222	0.0004
161	1	10	5	5	0	9	5	4	5296.2652	5296.26526	-0.0001
162	1	3	1	2	0	2	1	1	5296.3348	5296.33407	0.0007
163	1	4	2	3	0	3	2	2	5296.3403	5296.34155	-0.0013
164	1	8	4	4	0	7	4	3	5296.4361	5296.43659	-0.0005
165	1	6	3	3	0	5	3	2	5296.4627	5296.46231	0.0004
166	1	11	5	6	0	10	5	5	5296.5399	5296.53952	0.0004
167	1	4	1	3	0	3	1	2	5296.591	5296.59159	-0.0006
168	1	5	2	4	0	4	2	3	5296.5974	5296.59876	-0.0014
169	1	9	4	5	0	8	4	4	5296.7057	5296.70518	0.0005
170	1	7	3	4	0	6	3	3	5296.726	5296.72523	0.0008
171	1	12	5	7	0	11	5	6	5296.8174	5296.8166	0.0008
172	1	5	1	5	0	4	1	4	5296.8222	5296.82178	0.0004
173	1	5	1	4	0	4	1	3	5296.8527	5296.85205	0.0006
174	1	6	2	5	0	5	2	4	5296.8581	5296.85878	-0.0007
175	1	10	4	6	0	9	4	5	5296.9759	5296.9766	-0.0007
176	1	8	3	5	0	7	3	4	5296.9918	5296.99099	0.0008
177	1	6	1	6	0	5	1	5	5297.0778	5297.07838	-0.0006
178	1	13	5	8	0	12	5	7	5297.0968	5297.09649	0.0003
179	1	6	1	5	0	5	1	4	5297.1147	5297.11546	-0.0008
180	1	7	2	6	0	6	2	5	5297.1223	5297.12162	0.0007
181	1	6	0	6	0	5	0	5	5297.1751	5297.17608	-0.001
182	1	11	4	7	0	10	4	6	5297.2513	5297.25084	0.0005
183	1	9	3	6	0	8	3	5	5297.2595	5297.25958	-0.0001
184	1	7	1	7	0	6	1	6	5297.3377	5297.33766	0

185	1	14	5	9	0	13	5	8	5297.3798	5297.37919	0.0006
186	1	7	1	6	0	6	1	5	5297.381	5297.38179	-0.0008
187	1	8	2	7	0	7	2	6	5297.3869	5297.38727	-0.0004
188	1	7	0	7	0	6	0	6	5297.4396	5297.43872	0.0009
189	1	12	4	8	0	11	4	7	5297.5266	5297.5279	-0.0013
190	1	10	3	7	0	9	3	6	5297.5301	5297.531	-0.0009
191	1	8	1	8	0	7	1	7	5297.6004	5297.59962	0.0008
192	1	8	1	7	0	7	1	6	5297.6513	5297.65105	0.0002
193	1	9	2	8	0	8	2	7	5297.6555	5297.65572	-0.0002
194	1	15	5	10	0	14	5	9	5297.6638	5297.66471	-0.0009
195	1	8	0	8	0	7	0	7	5297.703	5297.7041	-0.0011
196	1	11	3	8	0	10	3	7	5297.805	5297.80525	-0.0003
197	1	13	4	9	0	12	4	8	5297.808	5297.80778	0.0002
198	1	9	1	9	0	8	1	8	5297.8634	5297.86425	-0.0009
199	1	9	1	8	0	8	1	7	5297.9243	5297.92324	0.0011
200	1	10	2	9	0	9	2	8	5297.9279	5297.92698	0.0009
201	1	16	5	11	0	15	5	10	5297.9528	5297.95303	-0.0002
202	1	9	0	9	0	8	0	8	5297.9716	5297.9722	-0.0006
203	1	12	3	9	0	11	3	8	5298.0822	5298.08234	-0.0001
204	1	14	4	10	0	13	4	9	5298.0914	5298.09048	0.0009
205	1	10	1	10	0	9	1	9	5298.1322	5298.13155	0.0006
206	1	10	1	9	0	9	1	8	5298.1981	5298.19833	-0.0002
207	1	11	2	10	0	10	2	9	5298.2018	5298.20102	0.0008
208	1	10	0	10	0	9	0	9	5298.243	5298.24301	0
209	1	17	5	12	0	16	5	11	5298.2451	5298.24416	0.0009
210	1	13	3	10	0	12	3	9	5298.3635	5298.36225	0.0012
211	1	15	4	11	0	14	4	10	5298.3749	5298.376	-0.0011
212	1	11	1	11	0	10	1	10	5298.4013	5298.40151	-0.0002
213	1	11	1	10	0	10	1	9	5298.4759	5298.47633	-0.0004
214	1	12	2	11	0	11	2	10	5298.4779	5298.47785	0
215	1	11	0	11	0	10	0	10	5298.5173	5298.5165	0.0008
216	1	18	5	13	0	17	5	12	5298.5376	5298.53809	-0.0005
217	1	14	3	11	0	13	3	10	5298.6442	5298.645	-0.0008
218	1	16	4	12	0	15	4	11	5298.6653	5298.66432	0.001
219	1	12	1	12	0	11	1	11	5298.6743	5298.67411	0.0002
220	1	12	1	11	0	11	1	10	5298.7565	5298.75722	-0.0007
221	1	12	0	12	0	11	0	11	5298.7921	5298.79265	-0.0006
222	1	19	5	14	0	18	5	13	5298.8342	5298.83483	-0.0006
223	1	15	3	12	0	14	3	11	5298.9311	5298.93058	0.0005
224	1	13	1	13	0	12	1	12	5298.9504	5298.94937	0.001
225	1	17	4	13	0	16	4	12	5298.9549	5298.95547	-0.0006
226	1	14	2	13	0	13	2	12	5299.0393	5299.03985	-0.0005
227	1	13	1	12	0	12	1	11	5299.042	5299.04101	0.001
228	1	13	0	13	0	12	0	12	5299.0713	5299.07144	-0.0001
229	1	20	5	15	0	19	5	14	5299.1355	5299.13436	0.0011

230	1	16	3	13	0	15	3	12	5299.2203	5299.21899	0.0013
231	1	14	1	14	0	13	1	13	5299.2271	5299.22725	-0.0002
232	1	18	4	14	0	17	4	13	5299.249	5299.24942	-0.0004
233	1	15	2	14	0	14	2	13	5299.3239	5299.325	-0.0011
234	1	14	1	13	0	13	1	12	5299.3284	5299.32766	0.0007
235	1	14	0	14	0	13	0	13	5299.3541	5299.35285	0.0013
236	1	21	5	16	0	20	5	15	5299.4361	5299.43668	-0.0006
237	1	15	1	15	0	14	1	14	5299.5086	5299.50777	0.0008
238	1	17	3	14	0	16	3	13	5299.5104	5299.51023	0.0002
239	1	19	4	15	0	18	4	14	5299.547	5299.54617	0.0008
240	1	31	8	23	0	30	8	22	5299.5501	5299.5497	0.0004
241	1	16	2	15	0	15	2	14	5299.6142	5299.61291	0.0013
242	1	15	1	14	0	14	1	13	5299.616	5299.61719	-0.0012
243	1	15	0	15	0	14	0	14	5299.6368	5299.63684	0
244	1	22	5	17	0	21	5	16	5299.7416	5299.7418	-0.0002
245	1	16	1	16	0	15	1	15	5299.7917	5299.79091	0.0008
246	1	18	3	15	0	17	3	14	5299.8043	5299.80431	0
247	1	20	4	16	0	19	4	15	5299.8454	5299.84574	-0.0003
248	1	32	8	24	0	31	8	23	5299.8817	5299.8825	-0.0008
249	1	17	2	16	0	16	2	15	5299.9037	5299.90357	0.0001
250	1	16	1	15	0	15	1	14	5299.9089	5299.90958	-0.0007
251	1	16	0	16	0	15	0	15	5299.9239	5299.92341	0.0005
252	1	23	5	18	0	22	5	17	5300.0504	5300.0497	0.0007
253	1	17	1	17	0	16	1	16	5300.0762	5300.07666	-0.0005
254	1	19	3	16	0	18	3	15	5300.1025	5300.10121	0.0013
255	1	21	4	17	0	20	4	16	5300.149	5300.14811	0.0009
256	1	18	2	17	0	17	2	16	5300.1976	5300.19698	0.0006
257	1	17	1	16	0	16	1	15	5300.2048	5300.20481	0
258	1	17	0	17	0	16	0	16	5300.2114	5300.21252	-0.0011
259	1	33	8	25	0	32	8	24	5300.2185	5300.21804	0.0005
260	1	24	5	19	0	23	5	18	5300.3594	5300.3604	-0.001
261	1	18	1	18	0	17	1	17	5300.3637	5300.36501	-0.0013
262	1	20	3	17	0	19	3	16	5300.4011	5300.40095	0.0001
263	1	22	4	18	0	21	4	17	5300.4528	5300.45328	-0.0005
264	1	19	2	18	0	18	2	17	5300.4922	5300.49312	-0.0009
265	1	18	1	17	0	17	1	16	5300.5039	5300.50288	0.001
266	1	18	0	18	0	17	0	17	5300.5032	5300.50414	-0.0009
267	1	34	8	26	0	33	8	25	5300.5566	5300.55632	0.0003
268	1	19	1	19	0	18	1	18	5300.655	5300.65596	-0.001
269	1	25	5	20	0	24	5	19	5300.6735	5300.67387	-0.0004
270	1	21	3	18	0	20	3	17	5300.7028	5300.70353	-0.0007
271	1	31	7	24	0	30	7	23	5300.725	5300.72411	0.0009
272	1	23	4	19	0	22	4	18	5300.7621	5300.76125	0.0009
273	1	20	2	19	0	19	2	18	5300.793	5300.79199	0.001
274	1	19	0	19	0	18	0	18	5300.7971	5300.79825	-0.0012

275	1	19	1	18	0	18	1	17	5300.8035	5300.80378	-0.0003
276	1	35	8	27	0	34	8	26	5300.8984	5300.89733	0.0011
277	1	20	1	20	0	19	1	19	5300.9488	5300.94949	-0.0007
278	1	26	5	21	0	25	5	20	5300.9887	5300.99013	-0.0014
279	1	22	3	19	0	21	3	18	5301.0086	5301.00894	-0.0003
280	1	32	7	25	0	31	7	24	5301.0565	5301.05689	-0.0004
281	1	24	4	20	0	23	4	19	5301.0725	5301.07202	0.0005
282	1	21	2	20	0	20	2	19	5301.0933	5301.09358	-0.0003
283	1	20	0	20	0	19	0	19	5301.0956	5301.09483	0.0008
284	1	20	1	19	0	19	1	18	5301.1072	5301.10748	-0.0003
285	1	36	8	28	0	35	8	27	5301.2419	5301.24106	0.0008
286	1	21	1	21	0	20	1	20	5301.2445	5301.24561	-0.0011
287	1	27	5	22	0	26	5	21	5301.3097	5301.30917	0.0005
288	1	23	3	20	0	22	3	19	5301.3173	5301.31719	0.0001
289	1	25	4	21	0	24	4	20	5301.3856	5301.38558	0
290	1	33	7	26	0	32	7	25	5301.3919	5301.39242	-0.0005
291	1	21	0	21	0	20	0	20	5301.3944	5301.39385	0.0005
292	1	22	2	21	0	21	2	20	5301.3984	5301.39788	0.0005
293	1	21	1	20	0	20	1	19	5301.4135	5301.41399	-0.0005
294	1	22	1	22	0	21	1	21	5301.5441	5301.54429	-0.0002
295	1	37	8	29	0	36	8	28	5301.5866	5301.58752	-0.0009
296	1	24	3	21	0	23	3	20	5301.628	5301.62828	-0.0003
297	1	28	5	23	0	27	5	22	5301.6319	5301.63098	0.0009
298	1	22	0	22	0	21	0	21	5301.6958	5301.69528	0.0005
299	1	26	4	22	0	25	4	21	5301.7018	5301.70194	-0.0001
300	1	23	2	22	0	22	2	21	5301.7059	5301.70488	0.001
301	1	22	1	21	0	21	1	20	5301.7239	5301.72329	0.0006
302	1	34	7	27	0	33	7	26	5301.7309	5301.73069	0.0002
303	1	23	2	21	0	22	2	20	5301.7329	5301.73255	0.0003
304	1	23	1	23	0	22	1	22	5301.8465	5301.84553	0.001
305	1	38	8	30	0	37	8	29	5301.9367	5301.9367	0
306	1	25	3	22	0	24	3	21	5301.9414	5301.94222	-0.0008
307	1	29	5	24	0	28	5	23	5301.9543	5301.95556	-0.0013
308	1	23	0	23	0	22	0	22	5302.0002	5301.99909	0.0011
309	1	24	2	23	0	23	2	22	5302.0143	5302.01458	-0.0003
310	1	27	4	23	0	26	4	22	5302.0202	5302.0211	-0.0009
311	1	23	1	22	0	22	1	21	5302.0347	5302.03536	-0.0007
312	1	24	2	22	0	23	2	21	5302.0476	5302.04648	0.0011
313	1	35	7	28	0	34	7	27	5302.0717	5302.0717	0
314	1	32	6	26	0	31	6	25	5302.0796	5302.07845	0.0012
315	1	24	1	24	0	23	1	23	5302.148	5302.14933	-0.0013
316	1	26	3	23	0	25	3	22	5302.2596	5302.259	0.0006
317	1	30	5	25	0	29	5	24	5302.2818	5302.28292	-0.0011
318	1	39	8	31	0	38	8	30	5302.2883	5302.28859	-0.0003
319	1	24	0	24	0	23	0	23	5302.3049	5302.30527	-0.0004



320	1	25	2	24	0	24	2	23	5302.326	5302.32696	-0.001
321	1	28	4	24	0	27	4	23	5302.3423	5302.34304	-0.0007
322	1	24	1	23	0	23	1	22	5302.3513	5302.35019	0.0011
323	1	25	2	23	0	24	2	22	5302.3635	5302.36351	0
324	1	33	6	27	0	32	6	26	5302.4132	5302.414	-0.0008
325	1	36	7	29	0	35	7	28	5302.4152	5302.41544	-0.0002
326	1	25	1	25	0	24	1	24	5302.456	5302.45567	0.0003
327	1	27	3	24	0	26	3	23	5302.5778	5302.57863	-0.0008
328	1	31	5	26	0	30	5	25	5302.612	5302.61303	-0.001
329	1	25	0	25	0	24	0	24	5302.6141	5302.61378	0.0003
330	1	26	2	25	0	25	2	24	5302.6428	5302.64202	0.0008
331	1	40	8	32	0	39	8	31	5302.6421	5302.64319	-0.0011
332	1	25	1	24	0	24	1	23	5302.6678	5302.66776	0
333	1	26	2	24	0	25	2	23	5302.6842	5302.68367	0.0005
334	1	34	6	28	0	33	6	27	5302.752	5302.7523	-0.0003
335	1	37	7	30	0	36	7	29	5302.762	5302.7619	0.0001
336	1	26	1	26	0	25	1	25	5302.7648	5302.76454	0.0003
337	1	28	3	25	0	27	3	24	5302.9022	5302.90111	0.0011
338	1	26	0	26	0	25	0	25	5302.9236	5302.9246	-0.001
339	1	32	5	27	0	31	5	26	5302.9461	5302.94592	0.0002
340	1	27	2	26	0	26	2	25	5302.9594	5302.95975	-0.0003
341	1	26	1	25	0	25	1	24	5302.9886	5302.98806	0.0005
342	1	30	4	26	0	29	4	25	5302.994	5302.99528	-0.0013
343	1	41	8	33	0	40	8	32	5303.0013	5303.0005	0.0008
344	1	27	2	25	0	26	2	24	5303.007	5303.00695	0
345	1	27	1	27	0	26	1	26	5303.0755	5303.07594	-0.0004
346	1	35	6	29	0	34	6	28	5303.0944	5303.09335	0.0011
347	1	38	7	31	0	37	7	30	5303.1109	5303.11109	-0.0002
348	1	29	3	26	0	28	3	25	5303.226	5303.22645	-0.0004
349	1	27	0	27	0	26	0	26	5303.2388	5303.23771	0.0011
350	1	28	2	27	0	27	2	26	5303.2791	5303.28013	-0.001
351	1	33	5	28	0	32	5	27	5303.2817	5303.28156	0.0001
352	1	27	1	26	0	26	1	25	5303.3106	5303.31108	-0.0005
353	1	31	4	27	0	30	4	26	5303.3256	5303.32558	0
354	1	28	2	26	0	27	2	25	5303.3341	5303.33338	0.0007
355	1	42	8	34	0	41	8	33	5303.3597	5303.3605	-0.0008
356	1	28	1	28	0	27	1	27	5303.3893	5303.38985	-0.0006
357	1	36	6	30	0	35	6	29	5303.4376	5303.43713	0.0005
358	1	39	7	32	0	38	7	31	5303.4623	5303.463	-0.0007
359	1	28	0	28	0	27	0	27	5303.5527	5303.55309	-0.0004
360	1	30	3	27	0	29	3	26	5303.5554	5303.55464	0.0008
361	1	29	2	28	0	28	2	27	5303.602	5303.60315	-0.0012
362	1	34	5	29	0	33	5	28	5303.6209	5303.61995	0.0009
363	1	28	1	27	0	27	1	26	5303.6361	5303.63679	-0.0007
364	1	32	4	28	0	31	4	27	5303.6591	5303.65867	0.0004

365	1	29	2	27	0	28	2	26	5303.6628	5303.66294	-0.0001
366	1	29	1	29	0	28	1	28	5303.7073	5303.70628	0.001
367	1	43	8	35	0	42	8	34	5303.7219	5303.72321	-0.0013
368	1	37	6	31	0	36	6	30	5303.7835	5303.78364	-0.0001
369	1	40	7	33	0	39	7	32	5303.8165	5303.81762	-0.0011
370	1	29	0	29	0	28	0	28	5303.8717	5303.87072	0.001
371	1	31	3	28	0	30	3	27	5303.8868	5303.88571	0.0011
372	1	30	2	29	0	29	2	28	5303.9297	5303.92882	0.0009
373	1	35	5	30	0	34	5	29	5303.9612	5303.9611	0.0001
374	1	29	1	28	0	28	1	27	5303.9641	5303.96518	-0.0011
375	1	33	4	29	0	32	4	28	5303.9955	5303.99453	0.001
376	1	30	2	28	0	29	2	27	5303.9947	5303.99566	-0.001
377	1	30	1	30	0	29	1	29	5304.024	5304.0252	-0.0012
378	1	44	8	36	0	43	8	35	5304.0893	5304.0886	0.0007
379	1	41	7	34	0	40	7	33	5304.1743	5304.17495	-0.0006
380	1	30	0	30	0	29	0	29	5304.1909	5304.19057	0.0003
381	1	32	3	29	0	31	3	28	5304.2193	5304.21964	-0.0003
382	1	31	2	30	0	30	2	29	5304.2564	5304.2571	-0.0007
383	1	30	1	29	0	29	1	28	5304.2963	5304.29623	0.0001
384	1	36	5	31	0	35	5	30	5304.3059	5304.305	0.0009
385	1	31	2	29	0	30	2	28	5304.3309	5304.33152	-0.0006
386	1	34	4	30	0	33	4	29	5304.3333	5304.33317	0.0001
387	1	31	1	31	0	30	1	30	5304.3472	5304.3466	0.0006
388	1	45	8	37	0	44	8	36	5304.4568	5304.45667	0.0001
389	1	31	0	31	0	30	0	30	5304.5119	5304.51263	-0.0007
390	1	42	7	35	0	41	7	34	5304.534	5304.53499	-0.001
391	1	33	3	30	0	32	3	29	5304.5573	5304.55645	0.0008
392	1	32	2	31	0	31	2	30	5304.588	5304.58801	0
393	1	31	1	30	0	30	1	29	5304.6303	5304.62992	0.0004
394	1	37	5	32	0	36	5	31	5304.6521	5304.65165	0.0005
395	1	32	2	30	0	31	2	29	5304.6712	5304.67054	0.0007
396	1	35	4	31	0	34	4	30	5304.6748	5304.67459	0.0002
397	1	46	8	38	0	45	8	37	5304.8267	5304.82743	-0.0007
398	1	32	0	32	0	31	0	31	5304.8379	5304.83689	0.001
399	1	34	3	32	0	33	3	31	5304.8905	5304.89011	0.0004
400	1	34	3	31	0	33	3	30	5304.8952	5304.89614	-0.0009
401	1	43	7	36	0	42	7	35	5304.8979	5304.89772	0.0002
402	1	33	2	32	0	32	2	31	5304.9214	5304.92151	-0.0001
403	1	32	1	31	0	31	1	30	5304.9671	5304.96624	0.0009
404	1	33	1	33	0	32	1	32	5304.9981	5304.99686	0.0012
405	1	38	5	33	0	37	5	32	5305.0001	5305.00103	-0.0009
406	1	33	2	31	0	32	2	30	5305.0128	5305.01269	0.0001
407	1	36	4	32	0	35	4	31	5305.0196	5305.01878	0.0008
408	1	33	0	33	0	32	0	32	5305.1627	5305.16333	-0.0006
409	1	47	8	39	0	46	8	38	5305.2012	5305.20086	0.0003

410	1	35	3	33	0	34	3	32	5305.2307	5305.23166	-0.001
411	1	35	3	32	0	34	3	31	5305.2376	5305.23872	-0.0011
412	1	34	2	33	0	33	2	32	5305.258	5305.25761	0.0004
413	1	44	7	37	0	43	7	36	5305.2635	5305.26316	0.0003
414	1	33	1	32	0	32	1	31	5305.3064	5305.30516	0.0012
415	1	34	1	34	0	33	1	33	5305.3266	5305.32568	0.0009
416	1	39	5	34	0	38	5	33	5305.3524	5305.35316	-0.0008
417	1	34	2	32	0	33	2	31	5305.3584	5305.35799	0.0004
418	1	37	4	33	0	36	4	32	5305.366	5305.36575	0.0003
419	1	34	0	34	0	33	0	33	5305.4905	5305.49194	-0.0014
420	1	36	3	34	0	35	3	33	5305.5759	5305.57596	-0.0001
421	1	48	8	40	0	47	8	39	5305.5782	5305.57696	0.0012
422	1	36	3	33	0	35	3	32	5305.583	5305.5842	-0.0012
423	1	35	2	34	0	34	2	33	5305.5969	5305.5963	0.0006
424	1	45	7	38	0	44	7	37	5305.6307	5305.63128	-0.0006
425	1	34	1	33	0	33	1	32	5305.6455	5305.64666	-0.0012
426	1	35	1	35	0	34	1	34	5305.6581	5305.65696	0.0011
427	1	35	2	33	0	34	2	32	5305.7068	5305.70642	0.0004
428	1	40	5	35	0	39	5	34	5305.7088	5305.70803	0.0008
429	1	38	4	34	0	37	4	33	5305.7165	5305.71549	0.001
430	1	35	0	35	0	34	0	34	5305.8237	5305.82272	0.001
431	1	37	3	35	0	36	3	34	5305.9234	5305.92302	0.0004
432	1	37	3	34	0	36	3	33	5305.932	5305.93257	-0.0006
433	1	36	2	35	0	35	2	34	5305.9375	5305.93755	-0.0001
434	1	49	8	41	0	48	8	40	5305.9572	5305.95572	0.0015
435	1	35	1	34	0	34	1	33	5305.9918	5305.99072	0.0011
436	1	46	7	39	0	45	7	38	5306.0022	5306.00209	0.0001
437	1	36	2	34	0	35	2	33	5306.0591	5306.05796	0.0011
438	1	41	5	36	0	40	5	35	5306.0659	5306.06562	0.0003
439	1	39	4	35	0	38	4	34	5306.0685	5306.06799	0.0005
440	1	36	0	36	0	35	0	35	5306.1556	5306.15565	-0.0001
441	1	38	3	36	0	37	3	35	5306.2724	5306.27281	-0.0004
442	1	37	2	36	0	36	2	35	5306.2805	5306.28137	-0.0009
443	1	38	3	35	0	37	3	34	5306.285	5306.28386	0.0011
444	1	37	1	37	0	36	1	36	5306.3264	5306.32685	-0.0005
445	1	50	8	42	0	49	8	41	5306.3361	5306.33715	-0.001
446	1	47	7	40	0	46	7	39	5306.3764	5306.37558	0.0008
447	1	37	2	35	0	36	2	34	5306.4118	5306.41261	-0.0008
448	1	40	4	36	0	39	4	35	5306.422	5306.42327	-0.0013
449	1	42	5	37	0	41	5	36	5306.4264	5306.42595	0.0005
450	1	37	0	37	0	36	0	36	5306.4918	5306.49074	0.0011
451	1	39	3	37	0	38	3	36	5306.6252	5306.62534	-0.0001
452	1	38	2	37	0	37	2	36	5306.6271	5306.62773	-0.0006
453	1	39	3	36	0	38	3	35	5306.6387	5306.63807	0.0006
454	1	38	1	38	0	37	1	37	5306.6665	5306.66544	0.0011

455	1	37	1	36	0	36	1	35	5306.6854	5306.68642	-0.001
456	1	51	8	43	0	50	8	42	5306.7212	5306.72122	0
457	1	48	7	41	0	47	7	40	5306.7529	5306.75175	0.0011
458	1	38	2	36	0	37	2	35	5306.7694	5306.77036	-0.001
459	1	41	4	37	0	40	4	36	5306.7801	5306.78131	-0.0012
460	1	43	5	38	0	42	5	37	5306.7902	5306.789	0.0012
461	1	38	0	38	0	37	0	37	5306.8271	5306.82798	-0.0009
462	1	39	2	38	0	38	2	37	5306.9756	5306.97663	-0.001
463	1	40	3	38	0	39	3	37	5306.9812	5306.9806	0.0006
464	1	40	3	37	0	39	3	36	5306.9947	5306.99521	-0.0005
465	1	39	1	39	0	38	1	38	5307.007	5307.00646	0.0005
466	1	38	1	37	0	37	1	36	5307.0386	5307.03803	0.0006
467	1	52	8	44	0	51	8	43	5307.1092	5307.10795	0.0012
468	1	49	7	42	0	48	7	41	5307.1316	5307.13059	0.001
469	1	39	2	37	0	38	2	36	5307.1311	5307.13117	-0.0001
470	1	42	4	38	0	41	4	37	5307.1426	5307.14212	0.0005
471	1	39	0	39	0	38	0	38	5307.1664	5307.16737	-0.001
472	1	40	2	39	0	39	2	38	5307.3279	5307.32806	-0.0002
473	1	41	3	39	0	40	3	38	5307.3377	5307.33857	-0.0009
474	1	40	1	40	0	39	1	39	5307.3493	5307.34989	-0.0006
475	1	41	3	38	0	40	3	37	5307.3558	5307.35528	0.0005
476	1	39	1	38	0	38	1	37	5307.3923	5307.39209	0.0002
477	1	40	2	38	0	39	2	37	5307.4964	5307.49503	0.0014
478	1	53	8	45	0	52	8	44	5307.4968	5307.49732	-0.0005
479	1	43	4	39	0	42	4	38	5307.5049	5307.50569	-0.0008
480	1	40	0	40	0	39	0	39	5307.5084	5307.50892	-0.0005
481	1	50	7	43	0	49	7	42	5307.5132	5307.5121	0.0011
482	1	41	2	40	0	40	2	39	5307.6828	5307.682	0.0008
483	1	41	1	41	0	40	1	40	5307.695	5307.69573	-0.0007
484	1	42	3	40	0	41	3	39	5307.6981	5307.69926	-0.0012
485	1	42	3	39	0	41	3	38	5307.7175	5307.7183	-0.0008
486	1	40	1	39	0	39	1	38	5307.7476	5307.7486	-0.001
487	1	41	0	41	0	40	0	40	5307.8537	5307.85262	0.0011
488	1	41	2	39	0	40	2	38	5307.8618	5307.86192	-0.0001
489	1	44	4	40	0	43	4	39	5307.8708	5307.87202	-0.0012
490	1	54	8	46	0	53	8	45	5307.8885	5307.88932	-0.0008
491	1	51	7	44	0	50	7	43	5307.896	5307.89626	-0.0003
492	1	42	2	41	0	41	2	40	5308.039	5308.03844	0.0006
493	1	42	1	42	0	41	1	41	5308.0448	5308.04396	0.0008
494	1	43	3	41	0	42	3	40	5308.0618	5308.06265	-0.0009
495	1	43	3	40	0	42	3	39	5308.0834	5308.08428	-0.0009
496	1	41	1	40	0	40	1	39	5308.1069	5308.10752	-0.0006
497	1	42	0	42	0	41	0	41	5308.1996	5308.1985	0.0011
498	1	42	2	40	0	41	2	39	5308.2313	5308.23181	-0.0005
499	1	45	4	41	0	44	4	40	5308.2402	5308.24112	-0.0009

500	1	47	5	42	0	46	5	41	5308.2697	5308.26837	0.0013
501	1	52	7	45	0	51	7	44	5308.2833	5308.28309	0.0002
502	1	55	8	47	0	54	8	46	5308.2842	5308.28396	0.0002
503	1	43	1	43	0	42	1	42	5308.3943	5308.39459	-0.0003
504	1	43	2	42	0	42	2	41	5308.3964	5308.39737	-0.001
505	1	44	3	42	0	43	3	41	5308.4287	5308.42874	0
506	1	44	3	41	0	43	3	40	5308.4538	5308.45322	0.0006
507	1	42	1	41	0	41	1	40	5308.4675	5308.46883	-0.0013
508	1	43	0	43	0	42	0	42	5308.5458	5308.54654	-0.0007
509	1	43	2	41	0	42	2	40	5308.606	5308.60468	0.0013
510	1	46	4	42	0	45	4	41	5308.6116	5308.61297	-0.0014
511	1	48	5	43	0	47	5	42	5308.6439	5308.64499	-0.0011
512	1	53	7	46	0	52	7	45	5308.6722	5308.67256	-0.0004
513	1	56	8	48	0	55	8	47	5308.6799	5308.68122	-0.0013
514	1	44	1	44	0	43	1	43	5308.7486	5308.7476	0.001
515	1	44	2	43	0	43	2	42	5308.7595	5308.75878	0.0007
516	1	45	3	43	0	44	3	42	5308.7981	5308.79751	0.0006
517	1	45	3	42	0	44	3	41	5308.8249	5308.82514	-0.0002
518	1	43	1	42	0	42	1	41	5308.8324	5308.8325	-0.0001
519	1	44	0	44	0	43	0	43	5308.8967	5308.89676	-0.0001
520	1	44	2	42	0	43	2	41	5308.9809	5308.98049	0.0004
521	1	47	4	43	0	46	4	42	5308.9881	5308.98759	0.0005
522	1	49	5	44	0	48	5	43	5309.0238	5309.02431	-0.0005
523	1	54	7	47	0	53	7	46	5309.0654	5309.06468	0.0007
524	1	57	8	49	0	56	8	48	5309.0824	5309.0811	0.0013
525	1	45	1	45	0	44	1	44	5309.1021	5309.10299	-0.0009
526	1	45	2	44	0	44	2	43	5309.1226	5309.12265	-0.0001
527	1	46	3	44	0	45	3	43	5309.1689	5309.16895	0
528	1	44	1	43	0	43	1	42	5309.199	5309.19851	0.0005
529	1	46	3	43	0	45	3	42	5309.1989	5309.20006	-0.0012
530	1	45	0	45	0	44	0	44	5309.248	5309.24918	-0.0012
531	1	52	6	46	0	51	6	45	5309.3065	5309.30664	-0.0001
532	1	45	2	43	0	44	2	42	5309.3589	5309.35921	-0.0003
533	1	48	4	44	0	47	4	43	5309.3659	5309.36496	0.0009
534	1	50	5	45	0	49	5	44	5309.4057	5309.40633	-0.0006
535	1	55	7	48	0	54	7	47	5309.4593	5309.45944	-0.0001
536	1	46	1	46	0	45	1	45	5309.4605	5309.46075	-0.0003
537	1	58	8	50	0	57	8	49	5309.4841	5309.48359	0.0005
538	1	46	2	45	0	45	2	44	5309.4891	5309.48898	0.0001
539	1	47	3	45	0	46	3	44	5309.5428	5309.54305	-0.0003
540	1	45	1	44	0	44	1	43	5309.5671	5309.56681	0.0003
541	1	47	3	44	0	46	3	43	5309.5768	5309.57797	-0.0012
542	1	46	0	46	0	45	0	45	5309.6048	5309.6038	0.001
543	1	53	6	47	0	52	6	46	5309.6969	5309.69632	0.0006
544	1	46	2	44	0	45	2	43	5309.7411	5309.74082	0.0003

545	1	49	4	45	0	48	4	44	5309.7456	5309.7451	0.0005
546	1	51	5	46	0	50	5	45	5309.7904	5309.79105	-0.0006
547	1	47	1	47	0	46	1	46	5309.8206	5309.82087	-0.0003
548	1	56	7	49	0	55	7	48	5309.856	5309.85683	-0.0008
549	1	47	2	46	0	46	2	45	5309.8572	5309.85775	-0.0005
550	1	59	8	51	0	58	8	50	5309.888	5309.8887	-0.0007
551	1	48	3	46	0	47	3	45	5309.9205	5309.91981	0.0007
552	1	46	1	45	0	45	1	44	5309.9383	5309.93739	0.0009
553	1	48	3	45	0	47	3	44	5309.9591	5309.9589	0.0002
554	1	47	0	47	0	46	0	46	5309.9597	5309.96063	-0.0009
555	1	54	6	48	0	53	6	47	5310.0886	5310.08866	-0.0001
556	1	47	2	45	0	46	2	44	5310.126	5310.12528	0.0007
557	1	50	4	46	0	49	4	45	5310.1274	5310.12799	-0.0006
558	1	52	5	47	0	51	5	46	5310.1776	5310.17845	-0.0009
559	1	48	1	48	0	47	1	47	5310.1844	5310.18335	0.001
560	1	48	2	47	0	47	2	46	5310.2277	5310.22894	-0.0012
561	1	57	7	50	0	56	7	49	5310.2564	5310.25685	-0.0004
562	1	60	8	52	0	59	8	51	5310.2968	5310.2964	0.0004
563	1	49	3	47	0	48	3	46	5310.3004	5310.29921	0.0012
564	1	47	1	46	0	46	1	45	5310.3111	5310.31022	0.0009
565	1	48	0	48	0	47	0	47	5310.3208	5310.31969	0.0011
566	1	49	3	46	0	48	3	45	5310.3436	5310.34284	0.0008
567	1	55	6	49	0	54	6	48	5310.4823	5310.48366	-0.0014
568	1	51	4	48	0	50	4	47	5310.51	5310.51088	-0.0009
569	1	48	2	46	0	47	2	45	5310.5137	5310.51255	0.0012
570	1	51	4	47	0	50	4	46	5310.5145	5310.51364	0.0009
571	1	49	1	49	0	48	1	48	5310.5481	5310.54818	-0.0001
572	1	53	5	48	0	52	5	47	5310.569	5310.56854	0.0005
573	1	49	2	48	0	48	2	47	5310.6031	5310.60255	0.0005
574	1	58	7	51	0	57	7	50	5310.6585	5310.65949	-0.001
575	1	49	0	49	0	48	0	48	5310.6806	5310.68099	-0.0004
576	1	50	3	48	0	49	3	47	5310.681	5310.68124	-0.0002
577	1	48	1	47	0	47	1	46	5310.6851	5310.68526	-0.0002
578	1	61	8	53	0	60	8	52	5310.7077	5310.7067	0.001
579	1	50	3	47	0	49	3	46	5310.7309	5310.72983	0.0011
580	1	56	6	50	0	55	6	49	5310.8825	5310.8813	0.0012
581	1	52	4	49	0	51	4	48	5310.8986	5310.89886	-0.0003
582	1	52	4	48	0	51	4	47	5310.903	5310.90204	0.001
583	1	49	2	47	0	48	2	46	5310.9028	5310.9026	0.0002
584	1	50	1	50	0	49	1	49	5310.9157	5310.91536	0.0003
585	1	54	5	49	0	53	5	48	5310.9598	5310.96132	-0.0015
586	1	50	2	49	0	49	2	48	5310.9793	5310.97857	0.0007
587	1	50	0	50	0	49	0	49	5311.0451	5311.04454	0.0006
588	1	49	1	48	0	48	1	47	5311.0618	5311.06249	-0.0007
589	1	59	7	52	0	58	7	51	5311.0651	5311.06475	0.0003

590	1	51	3	49	0	50	3	48	5311.0654	5311.06589	-0.0005
591	1	62	8	54	0	61	8	53	5311.1192	5311.11958	-0.0004
592	1	57	6	51	0	56	6	50	5311.2826	5311.28158	0.001
593	1	51	1	51	0	50	1	50	5311.2845	5311.28487	-0.0004
594	1	53	4	50	0	52	4	49	5311.2892	5311.28954	-0.0003
595	1	53	4	49	0	52	4	48	5311.2919	5311.29321	-0.0013
596	1	50	2	48	0	49	2	47	5311.296	5311.29539	0.0006
597	1	55	5	50	0	54	5	49	5311.3566	5311.35677	-0.0002
598	1	51	2	50	0	50	2	49	5311.357	5311.35697	0
599	1	51	0	51	0	50	0	50	5311.4117	5311.41035	0.0014
600	1	50	1	49	0	49	1	48	5311.4423	5311.44187	0.0004
601	1	52	3	50	0	51	3	49	5311.4529	5311.45314	-0.0002
602	1	60	7	53	0	59	7	52	5311.4729	5311.47262	0.0003
603	1	52	3	49	0	51	3	48	5311.5133	5311.51294	0.0004
604	1	63	8	55	0	62	8	54	5311.5346	5311.53505	-0.0005
605	1	52	1	52	0	51	1	51	5311.6554	5311.65672	-0.0013
606	1	54	4	51	0	53	4	50	5311.6824	5311.68291	-0.0005
607	1	58	6	52	0	57	6	51	5311.6849	5311.6845	0.0004
608	1	54	4	50	0	53	4	49	5311.6857	5311.68713	-0.0014
609	1	51	2	49	0	50	2	48	5311.6904	5311.6909	-0.0005
610	1	52	2	51	0	51	2	50	5311.7364	5311.73775	-0.0014
611	1	56	5	51	0	55	5	50	5311.7536	5311.7549	-0.0013
612	1	52	0	52	0	51	0	51	5311.7784	5311.77843	0
613	1	51	1	50	0	50	1	49	5311.8229	5311.82337	-0.0005
614	1	53	3	51	0	52	3	50	5311.8433	5311.84299	0.0003
615	1	61	7	54	0	60	7	53	5311.8835	5311.8831	0.0004
616	1	53	3	50	0	52	3	49	5311.9086	5311.9091	-0.0005
617	1	64	8	56	0	63	8	55	5311.952	5311.9531	-0.0011
618	1	53	1	53	0	52	1	52	5312.0314	5312.03089	0.0005
619	1	55	4	52	0	54	4	51	5312.0797	5312.07898	0.0007
620	1	55	4	51	0	54	4	50	5312.0852	5312.08382	0.0014
621	1	52	2	50	0	51	2	49	5312.0889	5312.08908	-0.0002
622	1	59	6	53	0	58	6	52	5312.0899	5312.09006	-0.0002
623	1	53	2	52	0	52	2	51	5312.1198	5312.1209	-0.0011
624	1	53	0	53	0	52	0	52	5312.1498	5312.1488	0.001
625	1	57	5	52	0	56	5	51	5312.1548	5312.15569	-0.0009
626	1	52	1	51	0	51	1	50	5312.2075	5312.20697	0.0005
627	1	54	3	52	0	53	3	51	5312.2359	5312.23542	0.0005
628	1	62	7	55	0	61	7	54	5312.2962	5312.29618	0
629	1	54	3	51	0	53	3	50	5312.3083	5312.30833	0
630	1	54	1	54	0	53	1	53	5312.4065	5312.40738	-0.0009
631	1	56	4	53	0	55	4	52	5312.4791	5312.47773	0.0014
632	1	56	4	52	0	55	4	51	5312.4823	5312.48326	-0.001
633	1	53	2	51	0	52	2	50	5312.49	5312.4899	0.0001
634	1	54	2	53	0	53	2	52	5312.5073	5312.5064	0.0009

635	1	54	0	54	0	53	0	53	5312.5222	5312.52146	0.0007
636	1	58	5	53	0	57	5	52	5312.5583	5312.55916	-0.0009
637	1	53	1	52	0	52	1	51	5312.592	5312.59263	-0.0006
638	1	55	3	53	0	54	3	52	5312.6317	5312.63042	0.0013
639	1	55	3	52	0	54	3	51	5312.7109	5312.71064	0.0003
640	1	63	7	56	0	62	7	55	5312.7129	5312.71185	0.0011
641	1	55	1	55	0	54	1	54	5312.7862	5312.78619	0
642	1	57	4	54	0	56	4	53	5312.8803	5312.87915	0.0011
643	1	57	4	53	0	56	4	52	5312.8854	5312.88547	-0.0001
644	1	54	2	52	0	53	2	51	5312.8926	5312.89333	-0.0007
645	1	55	2	54	0	54	2	53	5312.8942	5312.89425	0
646	1	55	0	55	0	54	0	54	5312.8955	5312.89642	-0.0009
647	1	59	5	54	0	58	5	53	5312.9664	5312.96528	0.0011
648	1	54	1	53	0	53	1	52	5312.98	5312.98032	-0.0003
649	1	56	3	54	0	55	3	53	5313.0275	5313.02797	-0.0005
650	1	56	3	53	0	55	3	52	5313.1157	5313.11606	-0.0004
651	1	64	7	57	0	63	7	56	5313.1303	5313.1301	0.0002
652	1	56	1	56	0	55	1	55	5313.1674	5313.1673	0.0001
653	1	56	0	56	0	55	0	55	5313.273	5313.2737	-0.0007
654	1	58	4	55	0	57	4	54	5313.2834	5313.28325	0.0001
655	1	56	2	55	0	55	2	54	5313.2841	5313.28442	-0.0003
656	1	58	4	54	0	57	4	53	5313.2903	5313.29044	-0.0001
657	1	55	2	53	0	54	2	52	5313.2991	5313.29932	-0.0002
658	1	62	6	56	0	61	6	55	5313.3223	5313.32246	-0.0002
659	1	55	1	54	0	54	1	53	5313.3706	5313.37001	0.0006
660	1	60	5	55	0	59	5	54	5313.375	5313.37406	0.0009
661	1	57	3	55	0	56	3	54	5313.4271	5313.42806	-0.001
662	1	57	3	54	0	56	3	53	5313.5236	5313.52457	-0.001
663	1	57	1	57	0	56	1	56	5313.5507	5313.55072	0
664	1	57	0	57	0	56	0	56	5313.6535	5313.6533	0.0002
665	1	57	2	56	0	56	2	55	5313.6782	5313.67691	0.0013
666	1	59	4	56	0	58	4	55	5313.69	5313.69002	0
667	1	59	4	55	0	58	4	54	5313.6989	5313.69817	0.0007
668	1	56	2	54	0	55	2	53	5313.708	5313.70785	0.0001
669	1	56	1	55	0	55	1	54	5313.7604	5313.76168	-0.0013
670	1	61	5	56	0	60	5	55	5313.7856	5313.7855	0.0001
671	1	58	3	56	0	57	3	55	5313.8302	5313.83068	-0.0005
672	1	58	3	55	0	57	3	54	5313.9354	5313.93619	-0.0008
673	1	58	1	58	0	57	1	57	5313.9365	5313.93644	0.0001
674	1	58	0	58	0	57	0	57	5314.0361	5314.03523	0.0009
675	1	58	2	57	0	57	2	56	5314.0707	5314.0717	-0.001
676	1	60	4	57	0	59	4	56	5314.0997	5314.09944	0.0003
677	1	60	4	56	0	59	4	55	5314.1099	5314.10867	0.0012
678	1	57	2	55	0	56	2	54	5314.1189	5314.11888	0
679	1	57	1	56	0	56	1	55	5314.1563	5314.1553	0.001



680	1	59	3	57	0	58	3	56	5314.2351	5314.23581	-0.0007
681	1	59	1	59	0	58	1	58	5314.3243	5314.32445	-0.0002
682	1	59	3	56	0	58	3	55	5314.3515	5314.35093	0.0006
683	1	59	0	59	0	58	0	58	5314.4199	5314.41948	0.0004
684	1	59	2	58	0	58	2	57	5314.469	5314.46878	0.0002
685	1	61	4	58	0	60	4	57	5314.5125	5314.51151	0.001
686	1	61	4	57	0	60	4	56	5314.521	5314.52194	-0.0009
687	1	58	2	56	0	57	2	55	5314.5321	5314.53237	-0.0003
688	1	58	1	57	0	57	1	56	5314.552	5314.55083	0.0012
689	1	60	3	58	0	59	3	57	5314.6425	5314.64343	-0.0009
690	1	60	1	60	0	59	1	59	5314.7146	5314.71475	-0.0002
691	1	60	3	57	0	59	3	56	5314.7686	5314.76878	-0.0002
692	1	60	0	60	0	59	0	59	5314.806	5314.80608	-0.0001
693	1	60	2	59	0	59	2	58	5314.8684	5314.86814	0.0003
694	1	62	4	59	0	61	4	58	5314.9269	5314.92622	0.0007
695	1	62	4	58	0	61	4	57	5314.9376	5314.93799	-0.0004
696	1	59	1	58	0	58	1	57	5314.9486	5314.94826	0.0003
697	1	61	3	59	0	60	3	58	5315.0533	5315.05354	-0.0002
698	1	61	1	61	0	60	1	60	5315.1077	5315.10734	0.0004
699	1	61	3	58	0	60	3	57	5315.19	5315.18975	0.0003
700	1	61	0	61	0	60	0	60	5315.1938	5315.19502	-0.0012
701	1	61	2	60	0	60	2	59	5315.2685	5315.26977	-0.0013
702	1	63	4	60	0	62	4	59	5315.3427	5315.34357	-0.0009
703	1	60	1	59	0	59	1	58	5315.3475	5315.34755	0
704	1	63	4	59	0	62	4	58	5315.3568	5315.3568	0
705	1	60	2	58	0	59	2	57	5315.3671	5315.36662	0.0005
706	1	62	3	60	0	61	3	59	5315.4668	5315.46612	0.0007
707	1	62	1	62	0	61	1	61	5315.5018	5315.5022	-0.0004
708	1	62	0	62	0	61	0	61	5315.586	5315.58631	-0.0003
709	1	62	3	59	0	61	3	58	5315.6148	5315.61384	0.001
710	1	62	2	61	0	61	2	60	5315.6735	5315.67366	-0.0002
711	1	61	1	60	0	60	1	59	5315.7496	5315.74868	0.0009
712	1	64	4	61	0	63	4	60	5315.7627	5315.76354	-0.0008
713	1	64	4	60	0	63	4	59	5315.7779	5315.7784	-0.0005
714	1	61	2	59	0	60	2	58	5315.7878	5315.78732	0.0005
715	1	63	1	63	0	62	1	62	5315.9002	5315.89934	0.0009
716	1	63	0	63	0	62	0	62	5315.9811	5315.97994	0.0012
717	1	63	3	60	0	62	3	59	5316.0421	5316.04104	0.0011
718	1	63	2	62	0	62	2	61	5316.0806	5316.07979	0.0008
719	1	62	1	61	0	61	1	60	5316.1515	5316.15164	-0.0001
720	1	65	4	62	0	64	4	61	5316.186	5316.18613	-0.0001
721	1	65	4	61	0	64	4	60	5316.2022	5316.20278	-0.0006
722	1	62	2	60	0	61	2	59	5316.2111	5316.21034	0.0008
723	1	64	1	64	0	63	1	63	5316.2996	5316.29874	0.0009
724	1	64	0	64	0	63	0	63	5316.3753	5316.37592	-0.0006

725	1	64	3	61	0	63	3	60	5316.4708	5316.47135	-0.0006
726	1	64	2	63	0	63	2	62	5316.4878	5316.48815	-0.0003
727	1	63	1	62	0	62	1	61	5316.5555	5316.55639	-0.0009
728	1	66	4	63	0	65	4	62	5316.6122	5316.61133	0.0009
729	1	66	4	62	0	65	4	61	5316.6312	5316.62995	0.0013
730	1	63	2	61	0	62	2	60	5316.6346	5316.63566	-0.0011
731	1	65	1	65	0	64	1	64	5316.7	5316.70041	-0.0004
732	1	65	0	65	0	64	0	64	5316.7735	5316.77424	-0.0007
733	1	65	2	64	0	64	2	63	5316.8993	5316.89873	0.0006
734	1	65	3	62	0	64	3	61	5316.9055	5316.90477	0.0007
735	1	64	1	63	0	63	1	62	5316.9637	5316.96293	0.0008
736	1	67	4	64	0	66	4	63	5317.0383	5317.03913	-0.0008
737	1	67	4	63	0	66	4	62	5317.0595	5317.05991	-0.0004
738	1	64	2	62	0	63	2	61	5317.0628	5317.06326	-0.0005
739	1	66	1	66	0	65	1	65	5317.1034	5317.10434	-0.0009
740	1	66	0	66	0	65	0	65	5317.1755	5317.17492	0.0006
741	1	66	2	65	0	65	2	64	5317.3122	5317.31152	0.0007
742	1	66	3	63	0	65	3	62	5317.3405	5317.34128	-0.0008
743	1	65	1	64	0	64	1	63	5317.3713	5317.37123	0.0001
744	1	68	4	65	0	67	4	64	5317.4692	5317.46951	-0.0003
745	1	68	4	64	0	67	4	63	5317.4914	5317.49266	-0.0013
746	1	65	2	63	0	64	2	62	5317.4922	5317.49309	-0.0009
747	1	67	1	67	0	66	1	66	5317.5106	5317.51052	0.0001
748	1	67	0	67	0	66	0	66	5317.5771	5317.57794	-0.0008
749	1	67	2	66	0	66	2	65	5317.7269	5317.72651	0.0004
750	1	67	3	64	0	66	3	63	5317.7813	5317.78086	0.0004
751	1	66	1	65	0	65	1	64	5317.7812	5317.78129	-0.0001
752	1	69	4	66	0	68	4	65	5317.9026	5317.90247	0.0001
753	1	68	1	68	0	67	1	67	5317.9179	5317.91895	-0.0011
754	1	66	2	64	0	65	2	63	5317.9254	5317.92513	0.0003
755	1	69	4	65	0	68	4	64	5317.9282	5317.92822	0
756	1	68	0	68	0	67	0	67	5317.9832	5317.9833	-0.0001
757	1	68	2	67	0	67	2	66	5318.1427	5318.14368	-0.001
758	1	69	1	69	0	68	1	68	5318.3308	5318.32963	0.0012
759	1	70	4	67	0	69	4	66	5318.3387	5318.338	0.0007
760	1	67	2	65	0	66	2	64	5318.3604	5318.35934	0.0011
761	1	70	4	66	0	69	4	65	5318.3663	5318.36658	-0.0003
762	1	69	0	69	0	68	0	68	5318.3912	5318.39101	0.0002
763	1	68	1	67	0	67	1	66	5318.6066	5318.60662	0
764	1	70	1	70	0	69	1	69	5318.7419	5318.74255	-0.0006
765	1	68	2	66	0	67	2	65	5318.7956	5318.79569	-0.0001
766	1	70	0	70	0	69	0	69	5318.8022	5318.80105	0.0011
767	1	69	1	68	0	68	1	67	5319.0227	5319.02188	0.0008
768	1	69	2	67	0	68	2	66	5319.233	5319.23415	-0.0012

B.6  $^{79}\text{BrNO } 2\nu_1 + \nu_3$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu'$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	62	8	54	0	63	8	55	3804.0595	3804.05955	-0.0001
2	1	62	8	54	0	63	8	55	3804.0589	3804.05955	-0.0007
3	1	61	8	53	0	62	8	54	3804.255	3804.25503	0
4	1	61	8	53	0	62	8	54	3804.2544	3804.25503	-0.0006
5	1	58	8	50	0	59	8	51	3804.8476	3804.84628	0.0013
6	1	58	8	50	0	59	8	51	3804.8461	3804.84628	-0.0002
7	1	63	7	56	0	64	7	57	3804.9018	3804.90203	-0.0002
8	1	63	7	56	0	64	7	57	3804.9022	3804.90203	0.0002
9	1	57	8	49	0	58	8	50	3805.0457	3805.04496	0.0007
10	1	57	8	49	0	58	8	50	3805.0449	3805.04496	-0.0001
11	1	62	7	55	0	63	7	56	3805.0967	3805.09674	0
12	1	61	7	54	0	62	7	55	3805.2916	3805.29224	-0.0006
13	1	54	8	46	0	55	8	47	3805.6455	3805.64583	-0.0003
14	1	54	8	46	0	55	8	47	3805.6459	3805.64583	0.0001
15	1	53	8	45	0	54	8	46	3805.8476	3805.84773	-0.0001
16	1	58	7	51	0	59	7	52	3805.8841	3805.88356	0.0005
17	1	58	7	51	0	59	7	52	3805.8832	3805.88356	-0.0004
18	1	69	4	66	0	70	4	67	3806.0471	3806.04749	-0.0004
19	1	69	4	65	0	70	4	66	3806.0532	3806.05303	0.0002
20	1	68	4	65	0	69	4	66	3806.2377	3806.23713	0.0006
21	1	68	4	64	0	69	4	65	3806.2425	3806.24198	0.0005
22	1	67	4	63	0	68	4	64	3806.431	3806.43181	-0.0008
23	1	54	7	47	0	55	7	48	3806.6824	3806.68323	-0.0008
24	1	54	7	47	0	55	7	48	3806.6845	3806.68323	0.0013
25	1	65	4	62	0	66	4	63	3806.8107	3806.81086	-0.0002
26	1	65	4	61	0	66	4	62	3806.8149	3806.81407	0.0008
27	1	69	1	68	0	70	1	69	3807.0066	3807.0072	-0.0006
28	1	69	1	69	0	70	1	70	3807.0609	3807.061	-0.0001
29	1	68	2	66	0	69	2	67	3807.1004	3807.09933	0.0011
30	1	66	3	63	0	67	3	64	3807.1338	3807.13394	-0.0001
31	1	60	5	55	0	61	5	56	3807.1569	3807.15554	0.0014
32	1	63	4	60	0	64	4	61	3807.1981	3807.19739	0.0007
33	1	63	4	59	0	64	4	60	3807.1993	3807.19979	-0.0005
34	1	68	1	67	0	69	1	68	3807.2025	3807.2014	0.0011
35	1	68	1	68	0	69	1	69	3807.2566	3807.25603	0.0006
36	1	46	8	38	0	47	8	39	3807.2842	3807.2836	0.0006
37	1	65	3	62	0	66	3	63	3807.3234	3807.32338	0
38	1	66	2	65	0	67	2	66	3807.424	3807.42456	-0.0006
39	1	66	2	64	0	67	2	65	3807.4785	3807.47858	-0.0001
40	1	61	4	58	0	62	4	59	3807.5864	3807.58717	-0.0008
41	1	61	4	57	0	62	4	58	3807.5888	3807.58893	-0.0001

42	1	65	2	64	0	66	2	65	3807.6204	3807.61952	0.0009
43	1	66	1	66	0	67	1	67	3807.6483	3807.64796	0.0003
44	1	66	0	66	0	67	0	67	3807.6683	3807.66855	-0.0003
45	1	65	2	63	0	66	2	64	3807.6689	3807.6693	-0.0004
46	1	63	3	60	0	64	3	61	3807.7038	3807.70517	-0.0014
47	1	60	4	57	0	61	4	58	3807.7831	3807.78328	-0.0002
48	1	60	4	56	0	61	4	57	3807.7844	3807.78478	-0.0004
49	1	65	1	64	0	66	1	65	3807.7864	3807.78711	-0.0007
50	1	65	1	65	0	66	1	66	3807.8437	3807.84486	-0.0012
51	1	64	2	62	0	65	2	63	3807.8613	3807.86075	0.0005
52	1	65	0	65	0	66	0	66	3807.8663	3807.86618	0.0001
53	1	63	2	62	0	64	2	63	3808.0125	3808.01143	0.0011
54	1	64	1	64	0	65	1	65	3808.0418	3808.04239	-0.0006
55	1	63	2	61	0	64	2	62	3808.0526	3808.05296	-0.0004
56	1	64	0	64	0	65	0	65	3808.0653	3808.06445	0.0009
57	1	61	3	59	0	62	3	60	3808.0708	3808.07181	-0.001
58	1	61	3	58	0	62	3	59	3808.0901	3808.09084	-0.0007
59	1	42	8	34	0	43	8	35	3808.1213	3808.12186	-0.0006
60	1	42	8	34	0	43	8	35	3808.1223	3808.12186	0.0004
61	1	63	1	62	0	64	1	63	3808.181	3808.18023	0.0008
62	1	63	1	63	0	64	1	64	3808.2406	3808.24056	0
63	1	63	0	63	0	64	0	64	3808.2633	3808.26334	0
64	1	60	3	58	0	61	3	59	3808.2687	3808.26837	0.0003
65	1	60	3	57	0	61	3	58	3808.2852	3808.28513	0.0001
66	1	54	5	49	0	55	5	50	3808.3504	3808.34984	0.0006
67	1	61	2	60	0	62	2	61	3808.4069	3808.406	0.0009
68	1	61	2	59	0	62	2	60	3808.4395	3808.43969	-0.0002
69	1	40	8	32	0	41	8	33	3808.5452	3808.54584	-0.0006
70	1	40	8	32	0	41	8	33	3808.5467	3808.54584	0.0009
71	1	53	5	48	0	54	5	49	3808.5518	3808.55174	0.0001
72	1	61	1	60	0	62	1	61	3808.5757	3808.57557	0.0001
73	1	60	2	59	0	61	2	60	3808.6051	3808.60429	0.0008
74	1	60	2	58	0	61	2	59	3808.6345	3808.63423	0.0003
75	1	61	1	61	0	62	1	62	3808.6399	3808.63878	0.0011
76	1	52	5	47	0	53	5	48	3808.7535	3808.75446	-0.001
77	1	60	1	59	0	61	1	60	3808.774	3808.77409	-0.0001
78	1	59	2	58	0	60	2	59	3808.8038	3808.80326	0.0005
79	1	59	2	57	0	60	2	58	3808.8304	3808.82957	0.0008
80	1	60	1	60	0	61	1	61	3808.8386	3808.83884	-0.0002
81	1	60	0	60	0	61	0	61	3808.8628	3808.86381	-0.001
82	1	38	8	30	0	39	8	31	3808.9734	3808.97304	0.0004
83	1	59	1	58	0	60	1	59	3808.9727	3808.9732	-0.0005
84	1	59	1	59	0	60	1	60	3809.0388	3809.03955	-0.0007
85	1	59	0	59	0	60	0	60	3809.0655	3809.06523	0.0003
86	1	49	5	44	0	50	5	45	3809.3677	3809.36748	0.0002

87	1	52	4	49	0	53	4	50	3809.3812	3809.38159	-0.0004
88	1	52	4	48	0	53	4	49	3809.383	3809.38192	0.0011
89	1	54	3	52	0	55	3	53	3809.4634	3809.46402	-0.0006
90	1	54	3	51	0	55	3	52	3809.4696	3809.47082	-0.0012
91	1	53	3	51	0	54	3	52	3809.6663	3809.66603	0.0003
92	1	53	3	50	0	54	3	51	3809.6707	3809.67171	-0.001
93	1	54	1	53	0	55	1	54	3809.9789	3809.97791	0.001
94	1	46	5	41	0	47	5	42	3809.9878	3809.98782	0
95	1	49	4	45	0	50	4	46	3809.9949	3809.99462	0.0003
96	1	54	1	54	0	55	1	55	3810.0522	3810.05267	-0.0005
97	1	54	0	54	0	55	0	55	3810.0829	3810.08167	0.0012
98	1	53	1	53	0	54	1	54	3810.2578	3810.25723	0.0006
99	1	53	0	53	0	54	0	54	3810.2861	3810.28682	-0.0007
100	1	49	3	47	0	50	3	48	3810.4815	3810.48206	-0.0006
101	1	49	3	46	0	50	3	47	3810.4838	3810.4844	-0.0006
102	1	46	4	42	0	47	4	43	3810.6142	3810.61475	-0.0005
103	1	51	1	51	0	52	1	52	3810.6685	3810.6683	0.0002
104	1	51	0	51	0	52	0	52	3810.6991	3810.69899	0.0001
105	1	42	5	37	0	43	5	38	3810.8266	3810.82629	0.0003
106	1	49	2	47	0	50	2	48	3810.8294	3810.82897	0.0004
107	1	49	2	48	0	50	2	49	3810.832	3810.83132	0.0007
108	1	50	1	50	0	51	1	51	3810.8737	3810.87481	-0.0011
109	1	50	0	50	0	51	0	51	3810.9062	3810.906	0.0002
110	1	49	1	48	0	50	1	49	3810.9976	3810.99901	-0.0014
111	1	49	1	49	0	50	1	50	3811.0821	3811.08199	0.0001
112	1	46	3	44	0	47	3	45	3811.1027	3811.10248	0.0002
113	1	46	3	43	0	47	3	44	3811.103	3811.10331	-0.0003
114	1	49	0	49	0	50	0	50	3811.1134	3811.11363	-0.0002
115	1	43	4	39	0	44	4	40	3811.2413	3811.24228	-0.001
116	1	47	2	46	0	48	2	47	3811.2464	3811.24553	0.0009
117	1	40	5	35	0	41	5	36	3811.2513	3811.25039	0.0009
118	1	36	6	30	0	37	6	31	3811.3425	3811.34338	-0.0009
119	1	47	1	46	0	48	1	47	3811.412	3811.41236	-0.0004
120	1	46	2	44	0	47	2	45	3811.4455	3811.44584	-0.0003
121	1	42	4	38	0	43	4	39	3811.4538	3811.45309	0.0007
122	1	46	2	45	0	47	2	46	3811.453	3811.45373	-0.0007
123	1	47	1	47	0	48	1	48	3811.4977	3811.49831	-0.0006
124	1	47	0	47	0	48	0	48	3811.5303	3811.53075	-0.0004
125	1	35	6	29	0	36	6	30	3811.5595	3811.55985	-0.0004
126	1	46	1	45	0	47	1	46	3811.6197	3811.62013	-0.0004
127	1	41	4	37	0	42	4	38	3811.6649	3811.66472	0.0002
128	1	38	5	33	0	39	5	34	3811.6777	3811.67771	0
129	1	46	1	46	0	47	1	47	3811.7074	3811.70747	-0.0001
130	1	43	3	40	0	44	3	41	3811.7308	3811.73009	0.0007
131	1	43	3	41	0	44	3	42	3811.7298	3811.73016	-0.0004

132	1	46	0	46	0	47	0	47	3811.7401	3811.74023	-0.0001
133	1	34	6	28	0	35	6	29	3811.7777	3811.77713	0.0006
134	1	45	1	44	0	46	1	45	3811.8273	3811.82865	-0.0014
135	1	40	4	36	0	41	4	37	3811.8765	3811.87717	-0.0007
136	1	42	3	39	0	43	3	40	3811.9411	3811.94074	0.0004
137	1	42	3	40	0	43	3	41	3811.9405	3811.941	-0.0005
138	1	33	6	27	0	34	6	28	3811.9955	3811.99521	0.0003
139	1	43	2	41	0	44	2	42	3812.0712	3812.07087	0.0003
140	1	43	2	42	0	44	2	43	3812.082	3812.08278	-0.0008
141	1	36	5	31	0	37	5	32	3812.1078	3812.10827	-0.0005
142	1	41	3	38	0	42	3	39	3812.1519	3812.15224	-0.0003
143	1	41	3	39	0	42	3	40	3812.1528	3812.15265	0.0001
144	1	43	1	42	0	44	1	43	3812.2476	3812.24796	-0.0004
145	1	42	2	40	0	43	2	41	3812.2815	3812.28103	0.0005
146	1	42	2	41	0	43	2	42	3812.2928	3812.29396	-0.0012
147	1	38	4	34	0	39	4	35	3812.3039	3812.30449	-0.0006
148	1	35	5	30	0	36	5	31	3812.3248	3812.32476	0
149	1	43	1	43	0	44	1	44	3812.3398	3812.33893	0.0009
150	1	40	3	37	0	41	3	38	3812.3652	3812.36458	0.0006
151	1	40	3	38	0	41	3	39	3812.3653	3812.36511	0.0002
152	1	43	0	43	0	44	0	44	3812.3727	3812.37243	0.0003
153	1	42	1	41	0	43	1	42	3812.4579	3812.45877	-0.0009
154	1	41	2	39	0	42	2	40	3812.492	3812.49211	-0.0001
155	1	41	2	40	0	42	2	41	3812.5053	3812.50589	-0.0006
156	1	34	5	29	0	35	5	30	3812.5423	3812.54205	0.0003
157	1	42	1	42	0	43	1	43	3812.551	3812.55076	0.0002
158	1	42	0	42	0	43	0	43	3812.5839	3812.58441	-0.0005
159	1	41	1	40	0	42	1	41	3812.6698	3812.67036	-0.0006
160	1	40	2	39	0	41	2	40	3812.7199	3812.71858	0.0013
161	1	36	4	32	0	37	4	33	3812.7353	3812.73506	0.0002
162	1	33	5	28	0	34	5	29	3812.7599	3812.76014	-0.0002
163	1	41	1	41	0	42	1	42	3812.7631	3812.76326	-0.0002
164	1	41	0	41	0	42	0	42	3812.7971	3812.79702	0.0001
165	1	40	1	39	0	41	1	40	3812.882	3812.88275	-0.0007
166	1	40	1	40	0	41	1	41	3812.9761	3812.97644	-0.0003
167	1	40	0	40	0	41	0	41	3813.0099	3813.01028	-0.0004
168	1	36	3	33	0	37	3	34	3813.2227	3813.22234	0.0004
169	1	36	3	34	0	37	3	35	3813.2226	3813.22305	-0.0004
170	1	34	3	31	0	35	3	32	3813.6562	3813.65618	0
171	1	34	3	32	0	35	3	33	3813.6571	3813.65687	0.0002
172	1	33	3	31	0	34	3	32	3813.8759	3813.87499	0.0009
173	1	10	10	0	0	10	10	1	3815.5059	3815.50638	-0.0005
174	1	10	10	0	0	10	10	1	3815.5063	3815.50638	-0.0001
175	1	12	10	2	0	12	10	3	3815.5239	3815.52395	-0.0001
176	1	12	10	2	0	12	10	3	3815.5231	3815.52395	-0.0009

177	1	13	10	3	0	13	10	4	3815.5348	3815.53388	0.0009
178	1	13	10	3	0	13	10	4	3815.5354	3815.53388	0.0015
179	1	14	10	4	0	14	10	5	3815.544	3815.54457	-0.0006
180	1	14	10	4	0	14	10	5	3815.5446	3815.54457	0
181	1	15	10	5	0	15	10	6	3815.556	3815.55602	0
182	1	15	10	5	0	15	10	6	3815.5556	3815.55602	-0.0004
183	1	9	9	0	0	9	9	1	3816.8038	3816.80404	-0.0002
184	1	10	9	1	0	10	9	2	3816.8123	3816.81165	0.0006
185	1	12	9	3	0	12	9	4	3816.8293	3816.82916	0.0001
186	1	13	9	4	0	13	9	5	3816.8397	3816.83906	0.0006
187	1	14	9	5	0	14	9	6	3816.8495	3816.84971	-0.0002
188	1	15	9	6	0	15	9	7	3816.8609	3816.86111	-0.0002
189	1	16	9	7	0	16	9	8	3816.8727	3816.87328	-0.0006
190	1	9	8	1	0	9	8	2	3817.9763	3817.97605	0.0002
191	1	10	8	2	0	10	8	3	3817.9834	3817.98364	-0.0002
192	1	12	8	4	0	12	8	5	3818.001	3818.0011	-0.0001
193	1	13	8	5	0	13	8	6	3818.0111	3818.01096	0.0001
194	1	14	8	6	0	14	8	7	3818.0216	3818.02158	0
195	1	15	8	7	0	15	8	8	3818.0335	3818.03295	0.0005
196	1	7	7	0	0	7	7	1	3819.0001	3819.00054	-0.0004
197	1	8	7	1	0	8	7	2	3819.0066	3819.0066	0
198	1	10	7	3	0	10	7	4	3819.02	3819.02098	-0.001
199	1	12	7	5	0	12	7	6	3819.0382	3819.03839	-0.0002
200	1	6	6	0	0	6	6	1	3819.8968	3819.89677	0
201	1	7	6	1	0	7	6	2	3819.9013	3819.90206	-0.0008
202	1	8	6	2	0	8	6	3	3819.9077	3819.90811	-0.0004
203	1	10	6	4	0	10	6	5	3819.9222	3819.92246	-0.0003
204	1	13	6	7	0	13	6	8	3819.9493	3819.94964	-0.0003
205	1	5	5	0	0	5	5	1	3820.6571	3820.65686	0.0002
206	1	6	5	1	0	6	5	2	3820.6615	3820.66139	0.0001
207	1	7	5	2	0	7	5	3	3820.6656	3820.66667	-0.0011
208	1	8	5	3	0	8	5	4	3820.6728	3820.6727	0.0001
209	1	11	5	6	0	11	5	7	3820.6967	3820.69532	0.0014
210	1	4	4	0	0	4	4	1	3821.2802	3821.27991	0.0003
211	1	5	4	1	0	5	4	2	3821.2836	3821.28368	-0.0001
212	1	6	4	2	0	6	4	3	3821.289	3821.28819	0.0008
213	1	7	4	3	0	7	4	4	3821.2938	3821.29347	0.0003
214	1	8	4	4	0	8	4	5	3821.299	3821.29949	-0.0005
215	1	10	4	6	0	10	4	7	3821.3126	3821.3138	-0.0012
216	1	11	4	7	0	10	4	6	3824.012	3824.013	-0.001
217	1	13	4	9	0	12	4	8	3824.5202	3824.5209	-0.0007
218	1	14	4	10	0	13	4	9	3824.7757	3824.77594	-0.0002
219	1	13	3	10	0	12	3	9	3825.0082	3825.009	-0.0008
220	1	15	4	11	0	14	4	10	3825.0324	3825.03171	0.0007
221	1	18	5	13	0	17	5	12	3825.1764	3825.17708	-0.0007

222	1	14	3	11	0	13	3	10	3825.2634	3825.26407	-0.0007
223	1	16	4	12	0	15	4	11	3825.2871	3825.28821	-0.0011
224	1	15	3	12	0	14	3	11	3825.521	3825.51988	0.0011
225	1	17	4	13	0	16	4	12	3825.5455	3825.54543	0.0001
226	1	16	3	13	0	15	3	12	3825.7773	3825.77642	0.0009
227	1	18	4	14	0	17	4	13	3825.8033	3825.80337	-0.0001
228	1	31	8	23	0	30	8	22	3825.8965	3825.89621	0.0003
229	1	21	5	16	0	20	5	15	3825.955	3825.95521	-0.0002
230	1	15	1	15	0	14	1	14	3826.0272	3826.02656	0.0006
231	1	17	3	14	0	16	3	13	3826.0341	3826.03371	0.0004
232	1	16	2	15	0	15	2	14	3826.1232	3826.123	0.0002
233	1	15	1	14	0	14	1	13	3826.1241	3826.1251	-0.001
234	1	15	0	15	0	14	0	14	3826.1399	3826.14115	-0.0012
235	1	22	5	17	0	21	5	16	3826.2168	3826.216	0.0008
236	1	16	1	16	0	15	1	15	3826.2791	3826.27865	0.0004
237	1	18	3	15	0	17	3	14	3826.2925	3826.29174	0.0008
238	1	17	2	16	0	16	2	15	3826.3789	3826.37977	-0.0009
239	1	16	1	15	0	15	1	14	3826.3847	3826.38493	-0.0002
240	1	16	0	16	0	15	0	15	3826.3948	3826.39606	-0.0013
241	1	17	1	17	0	16	1	16	3826.5314	3826.53133	0.0001
242	1	21	4	17	0	20	4	16	3826.5821	3826.58149	0.0006
243	1	18	2	17	0	17	2	16	3826.6375	3826.6372	0.0003
244	1	17	1	16	0	16	1	15	3826.6467	3826.64547	0.0012
245	1	17	0	17	0	16	0	16	3826.6515	3826.65146	0
246	1	34	8	26	0	33	8	25	3826.7014	3826.70168	-0.0003
247	1	18	1	18	0	17	1	17	3826.7831	3826.78458	-0.0015
248	1	22	4	18	0	21	4	17	3826.8428	3826.8423	0.0005
249	1	19	2	18	0	18	2	17	3826.8954	3826.89529	0.0001
250	1	18	1	17	0	17	1	16	3826.9062	3826.90673	-0.0005
251	1	18	0	18	0	17	0	17	3826.908	3826.90734	0.0007
252	1	31	7	24	0	30	7	23	3826.9306	3826.93126	-0.0007
253	1	19	1	19	0	18	1	18	3827.0386	3827.0384	0.0002
254	1	23	4	19	0	22	4	18	3827.1042	3827.10381	0.0004
255	1	19	0	19	0	18	0	18	3827.163	3827.16367	-0.0007
256	1	19	1	18	0	18	1	17	3827.1696	3827.1687	0.0009
257	1	36	8	28	0	35	8	27	3827.2418	3827.24196	-0.0002
258	1	37	8	29	0	36	8	28	3827.5128	3827.51308	-0.0003
259	1	27	5	22	0	26	5	21	3827.5297	3827.53044	-0.0007
260	1	34	7	27	0	33	7	26	3827.7371	3827.73648	0.0006
261	1	38	8	30	0	37	8	29	3827.7844	3827.78484	-0.0004
262	1	22	1	22	0	21	1	21	3827.8023	3827.80321	-0.0009
263	1	23	2	22	0	22	2	21	3827.934	3827.9341	-0.0001
264	1	22	0	22	0	21	0	21	3827.9357	3827.93519	0.0005
265	1	23	2	21	0	22	2	20	3827.9593	3827.95809	0.0012
266	1	22	1	21	0	21	1	20	3827.9582	3827.95869	-0.0005



267	1	23	1	23	0	22	1	22	3828.0583	3828.05924	-0.0009
268	1	29	5	24	0	28	5	23	3828.0607	3828.06107	-0.0004
269	1	27	4	23	0	26	4	22	3828.1582	3828.15694	0.0013
270	1	23	0	23	0	22	0	22	3828.1937	3828.19313	0.0006
271	1	23	1	22	0	22	1	21	3828.224	3828.22336	0.0006
272	1	36	7	29	0	35	7	28	3828.2765	3828.27659	-0.0001
273	1	30	5	25	0	29	5	24	3828.328	3828.32741	0.0006
274	1	25	2	24	0	24	2	23	3828.4565	3828.45727	-0.0008
275	1	25	2	23	0	24	2	22	3828.4887	3828.4887	0
276	1	37	7	30	0	36	7	29	3828.5477	3828.54763	0.0001
277	1	31	5	26	0	30	5	25	3828.595	3828.59443	0.0006
278	1	41	8	33	0	40	8	32	3828.6034	3828.60396	-0.0006
279	1	29	4	25	0	28	4	24	3828.6871	3828.68771	-0.0006
280	1	25	0	25	0	24	0	24	3828.7095	3828.71007	-0.0006
281	1	38	7	31	0	37	7	30	3828.8208	3828.81931	0.0015
282	1	42	8	34	0	41	8	33	3828.8788	3828.87827	0.0005
283	1	30	4	26	0	29	4	25	3828.9538	3828.95414	-0.0003
284	1	31	4	27	0	30	4	26	3829.2215	3829.22127	0.0002
285	1	34	5	29	0	33	5	28	3829.3996	3829.39955	0
286	1	44	8	36	0	43	8	35	3829.4281	3829.42874	-0.0006
287	1	30	3	27	0	29	3	26	3829.4467	3829.44593	0.0008
288	1	41	7	34	0	40	7	33	3829.6375	3829.6382	-0.0007
289	1	31	3	28	0	30	3	27	3829.7145	3829.71365	0.0008
290	1	30	2	29	0	29	2	28	3829.776	3829.77569	0.0003
291	1	30	2	28	0	29	2	27	3829.8326	3829.83216	0.0004
292	1	30	1	30	0	29	1	29	3829.8661	3829.86599	0.0001
293	1	42	7	35	0	41	7	34	3829.9134	3829.91243	0.001
294	1	36	5	31	0	35	5	30	3829.9393	3829.93965	-0.0003
295	1	46	8	38	0	45	8	37	3829.9823	3829.98169	0.0006
296	1	30	0	30	0	29	0	29	3830.0082	3830.00768	0.0005
297	1	31	2	30	0	30	2	29	3830.0418	3830.04111	0.0007
298	1	30	1	29	0	29	1	28	3830.0934	3830.09351	-0.0001
299	1	31	2	29	0	30	2	28	3830.1041	3830.10377	0.0003
300	1	31	1	31	0	30	1	30	3830.1271	3830.12609	0.001
301	1	37	5	32	0	36	5	31	3830.2108	3830.21069	0.0001
302	1	47	8	39	0	46	8	38	3830.2589	3830.25908	-0.0002
303	1	31	0	31	0	30	0	30	3830.269	3830.26799	0.001
304	1	35	4	31	0	34	4	30	3830.2979	3830.29668	0.0012
305	1	31	1	30	0	30	1	29	3830.363	3830.36301	0
306	1	32	1	32	0	31	1	31	3830.386	3830.38667	-0.0007
307	1	44	7	37	0	43	7	36	3830.4628	3830.46278	0
308	1	38	5	33	0	37	5	32	3830.4828	3830.48239	0.0004
309	1	32	0	32	0	31	0	31	3830.5283	3830.52854	-0.0002
310	1	36	4	32	0	35	4	31	3830.5676	3830.56725	0.0004
311	1	35	3	33	0	34	3	32	3830.7858	3830.7863	-0.0005

312	1	35	3	32	0	34	3	31	3830.792	3830.79219	-0.0002
313	1	37	4	33	0	36	4	32	3830.8392	3830.8385	0.0007
314	1	46	7	39	0	45	7	38	3831.0165	3831.01559	0.0009
315	1	35	2	34	0	34	2	33	3831.1089	3831.1083	0.0006
316	1	38	4	34	0	37	4	33	3831.11	3831.11042	-0.0004
317	1	35	2	33	0	34	2	32	3831.1998	3831.19987	-0.0001
318	1	47	7	40	0	46	7	39	3831.2914	3831.29292	-0.0015
319	1	41	5	36	0	40	5	35	3831.3004	3831.30142	-0.001
320	1	35	0	35	0	34	0	34	3831.3125	3831.31153	0.001
321	1	36	2	35	0	35	2	34	3831.3757	3831.37643	-0.0007
322	1	36	1	36	0	35	1	35	3831.4343	3831.43364	0.0007
323	1	36	2	34	0	35	2	33	3831.4769	3831.47626	0.0006
324	1	36	0	36	0	35	0	35	3831.5721	3831.57296	-0.0009
325	1	42	5	37	0	41	5	36	3831.5757	3831.57572	0
326	1	40	4	36	0	39	4	35	3831.6568	3831.65632	0.0005
327	1	37	1	37	0	36	1	36	3831.6961	3831.69651	-0.0004
328	1	37	0	37	0	36	0	36	3831.8362	3831.8346	0.0016
329	1	41	4	37	0	40	4	36	3831.9309	3831.93028	0.0006
330	1	38	1	38	0	37	1	37	3831.9597	3831.95982	-0.0001
331	1	37	1	36	0	36	1	35	3831.9918	3831.99078	0.001
332	1	38	0	38	0	37	0	37	3832.0963	3832.09646	-0.0002
333	1	40	3	38	0	39	3	37	3832.1464	3832.1459	0.0005
334	1	42	4	38	0	41	4	37	3832.2064	3832.20491	0.0015
335	1	38	1	37	0	37	1	36	3832.2627	3832.2637	-0.001
336	1	41	3	39	0	40	3	38	3832.4208	3832.41975	0.0011
337	1	41	3	38	0	40	3	37	3832.4335	3832.43346	0
338	1	40	1	40	0	39	1	39	3832.4868	3832.48773	-0.0009
339	1	40	0	40	0	39	0	39	3832.6214	3832.62083	0.0006
340	1	42	3	40	0	41	3	39	3832.6937	3832.69423	-0.0005
341	1	42	3	39	0	41	3	38	3832.7105	3832.70982	0.0007
342	1	41	2	40	0	40	2	39	3832.7248	3832.72465	0.0002
343	1	41	1	41	0	40	1	40	3832.7522	3832.75231	-0.0001
344	1	44	4	40	0	43	4	39	3832.7567	3832.75618	0.0005
345	1	40	1	39	0	39	1	38	3832.8107	3832.8108	-0.0001
346	1	41	2	39	0	40	2	38	3832.8723	3832.87178	0.0005
347	1	42	2	41	0	41	2	40	3832.9958	3832.99574	0.0001
348	1	42	1	42	0	41	1	41	3833.0172	3833.01732	-0.0001
349	1	41	1	40	0	40	1	39	3833.085	3833.08492	0.0001
350	1	42	0	42	0	41	0	41	3833.1464	3833.1461	0.0003
351	1	42	2	40	0	41	2	39	3833.1542	3833.15345	0.0007
352	1	44	3	42	0	43	3	41	3833.2451	3833.24504	0.0001
353	1	44	3	41	0	43	3	40	3833.2646	3833.265	-0.0004
354	1	46	4	42	0	45	4	41	3833.3095	3833.31013	-0.0006
355	1	42	1	41	0	41	1	40	3833.3592	3833.3594	-0.0002
356	1	44	2	43	0	43	2	42	3833.5393	3833.53929	0

357	1	44	1	44	0	43	1	43	3833.5495	3833.54855	0.001
358	1	47	4	43	0	46	4	42	3833.5873	3833.5881	-0.0008
359	1	44	0	44	0	43	0	43	3833.6714	3833.67234	-0.0009
360	1	44	2	42	0	43	2	41	3833.7193	3833.71921	0.0001
361	1	46	3	44	0	45	3	43	3833.7976	3833.79826	-0.0007
362	1	46	3	43	0	45	3	42	3833.8239	3833.82352	0.0004
363	1	48	4	44	0	47	4	43	3833.8661	3833.86674	-0.0006
364	1	44	1	43	0	43	1	42	3833.9104	3833.90936	0.001
365	1	47	3	45	0	46	3	44	3834.0748	3834.07576	-0.001
366	1	47	3	44	0	46	3	43	3834.1032	3834.10405	-0.0009
367	1	54	6	48	0	53	6	47	3834.1502	3834.15057	-0.0004
368	1	47	1	47	0	46	1	46	3834.3479	3834.34837	-0.0005
369	1	48	3	46	0	47	3	45	3834.3542	3834.35384	0.0004
370	1	47	2	46	0	46	2	45	3834.3581	3834.35792	0.0002
371	1	48	3	45	0	47	3	44	3834.3856	3834.38544	0.0002
372	1	50	4	46	0	49	4	45	3834.4267	3834.42601	0.0007
373	1	55	6	49	0	54	6	48	3834.432	3834.4327	-0.0007
374	1	47	0	47	0	46	0	46	3834.4634	3834.46368	-0.0003
375	1	47	2	45	0	46	2	44	3834.5734	3834.57343	0
376	1	51	4	48	0	50	4	47	3834.704	3834.70441	-0.0004

B.7  $^{81}\text{BrNO } 2\nu_1 + \nu_3$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu''$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	62	8	54	0	63	8	55	3806.2517	3806.25197	-0.0003
2	1	61	8	53	0	62	8	54	3806.4461	3806.44579	0.0003
3	1	63	7	56	0	64	7	57	3806.6046	3806.60432	0.0003
4	1	60	8	52	0	61	8	53	3806.6403	3806.6404	-0.0001
5	1	60	8	52	0	61	8	53	3806.64	3806.6404	-0.0004
6	1	62	7	55	0	63	7	56	3806.797	3806.79739	-0.0004
7	1	59	8	51	0	60	8	52	3806.8366	3806.83581	0.0008
8	1	61	7	54	0	62	7	55	3806.9909	3806.99125	-0.0004
9	1	58	8	50	0	59	8	51	3807.0322	3807.03203	0.0002
10	1	58	8	50	0	59	8	51	3807.0319	3807.03203	-0.0001
11	1	69	1	68	0	70	1	69	3807.174	3807.17398	0
12	1	60	7	53	0	61	7	54	3807.1857	3807.18592	-0.0002
13	1	60	7	53	0	61	7	54	3807.1859	3807.18592	0
14	1	69	1	69	0	70	1	70	3807.2026	3807.20234	0.0003
15	1	69	0	69	0	70	0	70	3807.2116	3807.21227	-0.0007
16	1	57	8	49	0	58	8	50	3807.2293	3807.22904	0.0003
17	1	68	1	67	0	69	1	68	3807.3635	3807.36436	-0.0009
18	1	59	7	52	0	60	7	53	3807.3807	3807.38138	-0.0007
19	1	59	7	52	0	60	7	53	3807.381	3807.38138	-0.0004
20	1	68	1	68	0	69	1	69	3807.3947	3807.39513	-0.0004

21	1	68	0	68	0	69	0	69	3807.4058	3807.40532	0.0005
22	1	56	8	48	0	57	8	49	3807.4269	3807.42686	0
23	1	56	8	48	0	57	8	49	3807.4264	3807.42686	-0.0005
24	1	61	6	55	0	62	6	56	3807.4659	3807.46514	0.0008
25	1	67	2	66	0	68	2	67	3807.4693	3807.46946	-0.0002
26	1	67	2	65	0	68	2	66	3807.4951	3807.49542	-0.0003
27	1	58	7	51	0	59	7	52	3807.5779	3807.57764	0.0003
28	1	67	1	67	0	68	1	68	3807.5881	3807.58855	-0.0004
29	1	67	0	67	0	68	0	68	3807.5996	3807.599	0.0006
30	1	55	8	47	0	56	8	48	3807.6254	3807.62547	-0.0001
31	1	55	8	47	0	56	8	48	3807.6253	3807.62547	-0.0002
32	1	66	2	65	0	67	2	66	3807.6614	3807.66132	0.0001
33	1	65	3	62	0	66	3	63	3807.6934	3807.69283	0.0006
34	1	57	7	50	0	58	7	51	3807.7749	3807.7747	0.0002
35	1	65	2	63	0	66	2	64	3807.8726	3807.87272	-0.0001
36	1	64	3	61	0	65	3	62	3807.8833	3807.88273	0.0006
37	1	65	1	64	0	66	1	65	3807.9396	3807.93904	0.0006
38	1	65	1	65	0	66	1	66	3807.9771	3807.97729	-0.0002
39	1	53	8	45	0	54	8	46	3808.0246	3808.02512	-0.0005
40	1	53	8	45	0	54	8	46	3808.025	3808.02512	-0.0001
41	1	64	2	63	0	65	2	64	3808.0472	3808.04706	0.0001
42	1	58	6	52	0	59	6	53	3808.0525	3808.05158	0.0009
43	1	60	5	55	0	61	5	56	3808.0616	3808.06172	-0.0001
44	1	64	2	62	0	65	2	63	3808.0627	3808.06256	0.0001
45	1	63	3	60	0	64	3	61	3808.0734	3808.07356	-0.0002
46	1	64	1	64	0	65	1	65	3808.1726	3808.17263	0
47	1	52	8	44	0	53	8	45	3808.226	3808.22615	-0.0001
48	1	63	2	62	0	64	2	63	3808.241	3808.24096	0
49	1	57	6	51	0	58	6	52	3808.2476	3808.24867	-0.0011
50	1	59	5	54	0	60	5	55	3808.2577	3808.25717	0.0005
51	1	62	3	59	0	63	3	60	3808.265	3808.26531	-0.0003
52	1	54	7	47	0	55	7	48	3808.3705	3808.3707	-0.0002
53	1	60	4	57	0	61	4	58	3808.3914	3808.39109	0.0003
54	1	51	8	43	0	52	8	44	3808.4282	3808.42798	0.0002
55	1	51	8	43	0	52	8	44	3808.4278	3808.42798	-0.0002
56	1	62	2	61	0	63	2	62	3808.4348	3808.43556	-0.0008
57	1	62	2	60	0	63	2	61	3808.4443	3808.44467	-0.0004
58	1	56	6	50	0	57	6	51	3808.4459	3808.44656	-0.0007
59	1	58	5	53	0	59	5	54	3808.454	3808.45344	0.0006
60	1	61	3	58	0	62	3	59	3808.4583	3808.45798	0.0003
61	1	62	1	61	0	63	1	62	3808.5192	3808.51923	0
62	1	62	1	62	0	63	1	63	3808.5649	3808.56522	-0.0003
63	1	53	7	46	0	54	7	47	3808.5707	3808.57097	-0.0003
64	1	53	7	46	0	54	7	47	3808.5707	3808.57097	-0.0003
65	1	59	4	56	0	60	4	57	3808.5863	3808.5865	-0.0002

66	1	59	4	55	0	60	4	56	3808.587	3808.5869	0.0001
67	1	61	2	60	0	62	2	61	3808.6318	3808.63085	0.0009
68	1	61	2	59	0	62	2	60	3808.6372	3808.63696	0.0002
69	1	55	6	49	0	56	6	50	3808.6453	3808.64526	0
70	1	57	5	52	0	58	5	53	3808.6514	3808.65051	0.0009
71	1	52	7	45	0	53	7	46	3808.7716	3808.77205	-0.0005
72	1	52	7	45	0	53	7	46	3808.7721	3808.77205	0
73	1	58	4	55	0	59	4	56	3808.7825	3808.78272	-0.0002
74	1	58	4	54	0	59	4	55	3808.7841	3808.78303	0.0011
75	1	60	2	59	0	61	2	60	3808.8273	3808.82685	0.0005
76	1	59	3	57	0	60	3	58	3808.8421	3808.84174	0.0004
77	1	54	6	48	0	55	6	49	3808.8444	3808.84475	-0.0004
78	1	56	5	51	0	57	5	52	3808.8493	3808.8484	0.0009
79	1	60	1	59	0	61	1	60	3808.9096	3808.90921	0.0004
80	1	60	1	60	0	61	1	61	3808.9603	3808.96039	-0.0001
81	1	51	7	44	0	52	7	45	3808.9744	3808.97393	0.0005
82	1	51	7	44	0	52	7	45	3808.9745	3808.97393	0.0006
83	1	57	4	54	0	58	4	55	3808.9796	3808.97975	-0.0001
84	1	59	2	58	0	60	2	59	3809.0238	3809.02355	0.0003
85	1	59	2	57	0	60	2	58	3809.0246	3809.02405	0.0006
86	1	58	3	56	0	59	3	57	3809.0379	3809.03812	-0.0002
87	1	58	3	55	0	59	3	56	3809.0409	3809.04145	-0.0005
88	1	53	6	47	0	54	6	48	3809.0462	3809.04506	0.0011
89	1	59	1	58	0	60	1	59	3809.1055	3809.10519	0.0003
90	1	59	1	59	0	60	1	60	3809.1595	3809.15895	0.0006
91	1	56	4	53	0	57	4	54	3809.1774	3809.17759	-0.0002
92	1	56	4	52	0	57	4	53	3809.1778	3809.17777	0
93	1	58	2	56	0	59	2	57	3809.2195	3809.21886	0.0006
94	1	58	2	57	0	59	2	58	3809.2208	3809.22096	-0.0002
95	1	57	3	55	0	58	3	56	3809.2351	3809.2353	-0.0002
96	1	57	3	54	0	58	3	55	3809.2377	3809.23775	0
97	1	52	6	46	0	53	6	47	3809.2463	3809.24617	0.0001
98	1	54	5	49	0	55	5	50	3809.2456	3809.24659	-0.001
99	1	58	1	57	0	59	1	58	3809.3013	3809.30183	-0.0005
100	1	58	1	58	0	59	1	59	3809.3583	3809.35816	0.0001
101	1	55	4	52	0	56	4	53	3809.376	3809.37625	-0.0003
102	1	55	4	51	0	56	4	52	3809.3761	3809.37637	-0.0003
103	1	57	2	55	0	58	2	56	3809.4142	3809.41453	-0.0003
104	1	57	2	56	0	58	2	57	3809.4187	3809.41908	-0.0004
105	1	56	3	54	0	57	3	55	3809.4323	3809.43326	-0.001
106	1	53	5	48	0	54	5	49	3809.4471	3809.4469	0.0002
107	1	51	6	45	0	52	6	46	3809.4485	3809.44808	0.0004
108	1	57	1	56	0	58	1	57	3809.4984	3809.49916	-0.0008
109	1	57	1	57	0	58	1	58	3809.5583	3809.55803	0.0003
110	1	56	2	54	0	57	2	55	3809.6107	3809.61107	-0.0004

111	1	56	2	55	0	57	2	56	3809.6177	3809.61792	-0.0002
112	1	55	3	53	0	56	3	54	3809.6327	3809.63202	0.0007
113	1	55	3	52	0	56	3	53	3809.6334	3809.63303	0.0004
114	1	52	5	47	0	53	5	48	3809.6487	3809.64801	0.0007
115	1	56	1	55	0	57	1	56	3809.6965	3809.69717	-0.0007
116	1	53	4	49	0	54	4	50	3809.7758	3809.77605	-0.0002
117	1	53	4	50	0	54	4	51	3809.7763	3809.77601	0.0003
118	1	55	2	53	0	56	2	54	3809.808	3809.80847	-0.0005
119	1	55	2	54	0	56	2	55	3809.8182	3809.81748	0.0007
120	1	54	3	52	0	55	3	53	3809.8314	3809.83157	-0.0002
121	1	54	3	51	0	55	3	52	3809.832	3809.83201	0
122	1	51	5	46	0	52	5	47	3809.8501	3809.84994	0.0002
123	1	44	8	36	0	45	8	37	3809.8637	3809.86342	0.0003
124	1	44	8	36	0	45	8	37	3809.8634	3809.86342	0
125	1	55	1	54	0	56	1	55	3809.8962	3809.89589	0.0003
126	1	55	1	55	0	56	1	56	3809.9595	3809.95972	-0.0002
127	1	52	4	48	0	53	4	49	3809.9769	3809.97712	-0.0002
128	1	54	2	52	0	55	2	53	3810.007	3810.00675	0.0002
129	1	54	2	53	0	55	2	54	3810.0174	3810.01777	-0.0004
130	1	53	3	50	0	54	3	51	3810.0312	3810.03187	-0.0007
131	1	53	3	51	0	54	3	52	3810.0312	3810.03192	-0.0007
132	1	43	8	35	0	44	8	36	3810.0716	3810.07171	-0.0001
133	1	54	1	53	0	55	1	54	3810.0951	3810.09532	-0.0002
134	1	54	1	54	0	55	1	55	3810.1622	3810.16156	0.0006
135	1	53	2	51	0	54	2	52	3810.2066	3810.20591	0.0007
136	1	52	3	49	0	53	3	50	3810.2322	3810.2326	-0.0004
137	1	52	3	50	0	53	3	51	3810.2338	3810.23307	0.0007
138	1	42	8	34	0	43	8	35	3810.2808	3810.28081	0
139	1	42	8	34	0	43	8	35	3810.2807	3810.28081	-0.0001
140	1	53	1	52	0	54	1	53	3810.2956	3810.29547	0.0001
141	1	52	2	50	0	53	2	51	3810.4057	3810.40596	-0.0003
142	1	52	2	51	0	53	2	52	3810.421	3810.42054	0.0005
143	1	41	8	33	0	42	8	34	3810.4917	3810.49072	0.001
144	1	52	1	51	0	53	1	52	3810.496	3810.49635	-0.0003
145	1	52	1	52	0	53	1	53	3810.567	3810.56723	-0.0002
146	1	40	8	32	0	41	8	33	3810.7019	3810.70144	0.0005
147	1	39	8	31	0	40	8	32	3810.9127	3810.91297	-0.0003
148	1	39	8	31	0	40	8	32	3810.9128	3810.91297	-0.0002
149	1	44	4	40	0	45	4	41	3811.6155	3811.61509	0.0004
150	1	43	4	39	0	44	4	40	3811.8232	3811.8235	-0.0003
151	1	44	3	41	0	45	3	42	3811.8696	3811.86947	0.0001
152	1	44	3	42	0	45	3	43	3811.8714	3811.87125	0.0002
153	1	42	4	38	0	43	4	39	3812.0316	3812.03273	-0.0011
154	1	44	2	42	0	45	2	43	3812.0379	3812.03873	-0.0008
155	1	43	3	41	0	44	3	42	3812.0792	3812.07966	-0.0005

156	1	40	5	35	0	41	5	36	3812.1252	3812.12449	0.0007
157	1	41	4	37	0	42	4	38	3812.2421	3812.24276	-0.0007
158	1	43	2	41	0	44	2	42	3812.2469	3812.2469	0
159	1	42	3	39	0	43	3	40	3812.2866	3812.28713	-0.0005
160	1	42	3	40	0	43	3	41	3812.2888	3812.28887	-0.0001
161	1	41	3	38	0	42	3	39	3812.4969	3812.49721	-0.0003
162	1	41	3	39	0	42	3	40	3812.4986	3812.4989	-0.0003
163	1	38	5	33	0	39	5	34	3812.5484	3812.54854	-0.0001
164	1	36	6	30	0	37	6	31	3812.5739	3812.5736	0.0003
165	1	39	4	35	0	40	4	36	3812.6649	3812.66526	-0.0004
166	1	41	2	39	0	42	2	40	3812.6658	3812.66596	-0.0002
167	1	40	3	38	0	41	3	39	3812.7105	3812.70974	0.0008
168	1	35	6	29	0	36	6	30	3812.7892	3812.78841	0.0008
169	1	38	4	34	0	39	4	35	3812.8783	3812.87772	0.0006
170	1	40	2	39	0	41	2	40	3812.8995	3812.90005	-0.0005
171	1	39	3	36	0	40	3	37	3812.9206	3812.91983	0.0008
172	1	39	3	37	0	40	3	38	3812.9216	3812.9214	0.0002
173	1	38	3	36	0	39	3	37	3813.134	3813.13386	0.0001
174	1	33	6	27	0	34	6	28	3813.22	3813.22046	-0.0005
175	1	36	4	32	0	37	4	33	3813.3049	3813.30506	-0.0002
176	1	37	3	34	0	38	3	35	3813.3448	3813.34574	-0.0009
177	1	37	3	35	0	38	3	36	3813.3471	3813.34713	0
178	1	38	1	37	0	39	1	38	3813.3902	3813.3902	0
179	1	34	5	29	0	35	5	30	3813.406	3813.40631	-0.0003
180	1	32	6	26	0	33	6	27	3813.4372	3813.43769	-0.0005
181	1	38	1	38	0	39	1	39	3813.4824	3813.48251	-0.0001
182	1	35	4	31	0	36	4	32	3813.5195	3813.51994	-0.0004
183	1	36	3	33	0	37	3	34	3813.5594	3813.55991	-0.0005
184	1	37	1	36	0	38	1	37	3813.6029	3813.60302	-0.0001
185	1	31	6	25	0	32	6	26	3813.655	3813.65572	-0.0007
186	1	37	1	37	0	38	1	38	3813.6961	3813.6959	0.0002
187	1	35	3	33	0	36	3	34	3813.7766	3813.77609	0.0005
188	1	36	1	36	0	37	1	37	3813.9103	3813.91	0.0003
189	1	34	3	31	0	35	3	32	3813.9911	3813.99068	0.0004
190	1	34	3	32	0	35	3	33	3813.9925	3813.99179	0.0007
191	1	33	3	31	0	34	3	32	3814.2083	3814.20829	0
192	1	10	10	0	0	10	10	1	3818.7675	3818.76698	0.0005
193	1	10	10	0	0	10	10	1	3818.7671	3818.76698	0.0001
194	1	11	10	2	0	11	10	1	3818.7757	3818.77543	0.0003
195	1	11	10	1	0	11	10	2	3818.7751	3818.77543	-0.0003
196	1	12	10	2	0	12	10	3	3818.7839	3818.78464	-0.0007
197	1	12	10	2	0	12	10	3	3818.7851	3818.78464	0.0005
198	1	13	10	3	0	13	10	4	3818.7941	3818.79461	-0.0005
199	1	13	10	3	0	13	10	4	3818.7946	3818.79461	0
200	1	14	10	4	0	14	10	5	3818.8047	3818.80535	-0.0006

201	1	15	10	5	0	15	10	6	3818.8175	3818.81685	0.0007
202	1	11	9	2	0	11	9	3	3819.4634	3819.46346	-0.0001
203	1	12	9	3	0	12	9	4	3819.4732	3819.47263	0.0006
204	1	15	9	6	0	15	9	7	3819.505	3819.50472	0.0003
205	1	16	9	7	0	16	9	8	3819.5167	3819.51694	-0.0002
206	1	10	8	2	0	10	8	3	3820.0721	3820.07238	-0.0003
207	1	11	8	3	0	11	8	4	3820.0805	3820.08076	-0.0003
208	1	10	7	3	0	10	7	4	3820.6182	3820.61842	-0.0002
209	1	11	7	4	0	11	7	5	3820.6268	3820.62678	0
210	1	6	6	0	0	6	6	1	3821.0672	3821.06688	0.0003
211	1	10	6	4	0	10	6	5	3821.0934	3821.09267	0.0007
212	1	11	6	5	0	11	6	6	3821.1014	3821.10101	0.0004
213	1	12	6	6	0	12	6	7	3821.1096	3821.11011	-0.0005
214	1	13	6	7	0	13	6	8	3821.1191	3821.11996	-0.0009
215	1	5	5	0	0	5	5	1	3821.4654	3821.46441	0.001
216	1	6	5	1	0	6	5	2	3821.468	3821.46896	-0.001
217	1	11	5	6	0	11	5	7	3821.5032	3821.50302	0.0002
218	1	5	4	1	0	5	4	2	3821.7938	3821.79389	-0.0001
219	1	11	4	7	0	10	4	6	3824.5057	3824.50599	-0.0003
220	1	13	3	10	0	12	3	9	3825.2665	3825.26718	-0.0007
221	1	15	3	12	0	14	3	11	3825.7756	3825.77498	0.0006
222	1	16	3	13	0	15	3	12	3826.0296	3826.02998	-0.0004
223	1	15	0	15	0	14	0	14	3826.0983	3826.09822	0.0001
224	1	16	2	15	0	15	2	14	3826.2109	3826.21097	-0.0001
225	1	19	5	14	0	18	5	13	3826.2138	3826.21381	0
226	1	17	3	14	0	16	3	13	3826.2858	3826.28573	0.0001
227	1	17	2	16	0	16	2	15	3826.4656	3826.46624	-0.0006
228	1	20	5	15	0	19	5	14	3826.4721	3826.47166	0.0004
229	1	18	3	15	0	17	3	14	3826.5426	3826.54221	0.0004
230	1	17	0	17	0	16	0	16	3826.606	3826.60571	0.0003
231	1	19	3	16	0	18	3	15	3826.7992	3826.79944	-0.0002
232	1	19	2	18	0	18	2	17	3826.9794	3826.97877	0.0006
233	1	22	5	17	0	21	5	16	3826.9894	3826.9895	-0.0001
234	1	20	3	17	0	19	3	16	3827.058	3827.0574	0.0006
235	1	19	0	19	0	18	0	18	3827.1154	3827.11518	0.0002
236	1	20	2	19	0	19	2	18	3827.2357	3827.23603	-0.0003
237	1	23	5	18	0	22	5	17	3827.249	3827.24948	-0.0005
238	1	21	3	18	0	20	3	17	3827.3168	3827.3161	0.0007
239	1	20	0	20	0	19	0	19	3827.3708	3827.37062	0.0002
240	1	21	2	20	0	20	2	19	3827.4937	3827.49394	-0.0002
241	1	24	5	19	0	23	5	18	3827.51	3827.51017	-0.0002
242	1	21	0	21	0	20	0	20	3827.6259	3827.6265	-0.0006
243	1	22	2	21	0	21	2	20	3827.7524	3827.7525	-0.0001
244	1	23	3	20	0	22	3	19	3827.8359	3827.83572	0.0002
245	1	23	2	22	0	22	2	21	3828.011	3828.0117	-0.0007



246	1	26	5	21	0	25	5	20	3828.0335	3828.03363	-0.0001
247	1	24	2	23	0	23	2	22	3828.2717	3828.27153	0.0002
248	1	31	7	24	0	30	7	23	3828.4809	3828.48113	-0.0002
249	1	25	2	24	0	24	2	23	3828.5318	3828.53199	-0.0002
250	1	28	5	23	0	27	5	22	3828.5603	3828.55987	0.0004
251	1	25	2	23	0	24	2	22	3828.5608	3828.56096	-0.0002
252	1	26	3	23	0	25	3	22	3828.6214	3828.6207	0.0007
253	1	27	4	23	0	26	4	22	3828.6263	3828.62547	0.0008
254	1	26	2	25	0	25	2	24	3828.7924	3828.79306	-0.0007
255	1	29	5	24	0	28	5	23	3828.8245	3828.82403	0.0005
256	1	26	2	24	0	25	2	23	3828.8271	3828.82591	0.0012
257	1	27	3	24	0	26	3	23	3828.8844	3828.88385	0.0006
258	1	28	4	24	0	27	4	23	3828.8893	3828.88899	0.0003
259	1	33	7	26	0	32	7	25	3829.0141	3829.01433	-0.0002
260	1	27	2	26	0	26	2	25	3829.054	3829.05475	-0.0007
261	1	30	5	25	0	29	5	24	3829.0893	3829.08887	0.0004
262	1	32	6	26	0	31	6	25	3829.2195	3829.21975	-0.0002
263	1	34	7	27	0	33	7	26	3829.2821	3829.28192	0.0002
264	1	28	2	27	0	27	2	26	3829.3169	3829.31704	-0.0001
265	1	29	3	26	0	28	3	25	3829.412	3829.41237	-0.0004
266	1	30	4	26	0	29	4	25	3829.4174	3829.41813	-0.0007
267	1	35	7	28	0	34	7	27	3829.5505	3829.55018	0.0003
268	1	29	2	28	0	28	2	27	3829.5801	3829.57993	0.0002
269	1	29	2	27	0	28	2	26	3829.6266	3829.62645	0.0002
270	1	31	4	27	0	30	4	26	3829.6841	3829.68374	0.0004
271	1	34	6	28	0	33	6	27	3829.7541	3829.75417	-0.0001
272	1	29	1	28	0	28	1	27	3829.7942	3829.79344	0.0008
273	1	36	7	29	0	35	7	28	3829.8193	3829.8191	0.0002
274	1	30	1	30	0	29	1	29	3829.8361	3829.83567	0.0004
275	1	30	2	29	0	29	2	28	3829.8435	3829.8434	0.0001
276	1	33	5	28	0	32	5	27	3829.8879	3829.88747	0.0004
277	1	35	6	29	0	34	6	28	3830.0226	3830.02238	0.0002
278	1	37	7	30	0	36	7	29	3830.088	3830.08867	-0.0007
279	1	31	1	31	0	30	1	30	3830.0942	3830.09449	-0.0003
280	1	31	2	30	0	30	2	29	3830.1066	3830.10746	-0.0009
281	1	34	5	29	0	33	5	28	3830.1545	3830.15502	-0.0005
282	1	33	4	29	0	32	4	28	3830.2174	3830.21703	0.0004
283	1	31	1	30	0	30	1	29	3830.3297	3830.32922	0.0005
284	1	32	1	32	0	31	1	31	3830.3542	3830.35379	0.0004
285	1	32	2	31	0	31	2	30	3830.3721	3830.37209	0
286	1	32	2	30	0	31	2	29	3830.4364	3830.43551	0.0009
287	1	33	3	30	0	32	3	29	3830.4785	3830.47842	0.0001
288	1	34	4	30	0	33	4	29	3830.4848	3830.48471	0.0001
289	1	37	6	31	0	36	6	30	3830.5603	3830.56078	-0.0005
290	1	33	1	33	0	32	1	32	3830.614	3830.61358	0.0004

291	1	39	7	32	0	38	7	31	3830.6292	3830.62975	-0.0006
292	1	36	5	31	0	35	5	30	3830.6927	3830.69213	0.0006
293	1	33	2	31	0	32	2	30	3830.7066	3830.70708	-0.0005
294	1	34	3	31	0	33	3	30	3830.7465	3830.74682	-0.0003
295	1	35	4	31	0	34	4	30	3830.7528	3830.75307	-0.0003
296	1	33	1	32	0	32	1	31	3830.8678	3830.86725	0.0005
297	1	34	1	34	0	33	1	33	3830.8739	3830.87386	0
298	1	34	2	33	0	33	2	32	3830.9028	3830.90304	-0.0002
299	1	42	8	34	0	41	8	33	3830.9035	3830.90344	0.0001
300	1	37	5	32	0	36	5	31	3830.9617	3830.96168	0
301	1	34	2	32	0	33	2	31	3830.979	3830.97959	-0.0006
302	1	35	3	32	0	34	3	31	3831.0156	3831.01597	-0.0004
303	1	36	4	32	0	35	4	31	3831.0213	3831.02212	-0.0008
304	1	35	1	35	0	34	1	34	3831.1344	3831.1346	-0.0002
305	1	34	1	33	0	33	1	32	3831.1366	3831.13708	-0.0005
306	1	35	2	34	0	34	2	33	3831.1692	3831.16934	-0.0001
307	1	41	7	34	0	40	7	33	3831.174	3831.17341	0.0006
308	1	43	8	35	0	42	8	34	3831.1763	3831.17693	-0.0006
309	1	36	3	34	0	35	3	33	3831.2798	3831.27991	-0.0001
310	1	36	3	33	0	35	3	32	3831.2857	3831.2859	-0.0002
311	1	37	4	33	0	36	4	32	3831.2916	3831.29184	-0.0002
312	1	36	1	36	0	35	1	35	3831.3948	3831.39582	-0.001
313	1	35	1	34	0	34	1	33	3831.4082	3831.40743	0.0008
314	1	36	2	35	0	35	2	34	3831.4361	3831.43619	-0.0001
315	1	42	7	35	0	41	7	34	3831.4466	3831.44618	0.0004
316	1	36	2	34	0	35	2	33	3831.5276	3831.52737	0.0002
317	1	37	3	34	0	36	3	33	3831.5569	3831.55659	0.0003
318	1	37	1	37	0	36	1	36	3831.6578	3831.65749	0.0003
319	1	36	1	35	0	35	1	34	3831.6792	3831.67828	0.0009
320	1	43	7	36	0	42	7	35	3831.7196	3831.71959	0
321	1	45	8	37	0	44	8	36	3831.726	3831.72578	0.0002
322	1	40	5	35	0	39	5	34	3831.7738	3831.77428	-0.0005
323	1	37	2	35	0	36	2	34	3831.8029	3831.80262	0.0003
324	1	38	3	36	0	37	3	35	3831.8195	3831.82007	-0.0006
325	1	38	3	35	0	37	3	34	3831.8274	3831.82805	-0.0006
326	1	39	4	35	0	38	4	34	3831.833	3831.83332	-0.0003
327	1	38	1	38	0	37	1	37	3831.919	3831.91962	-0.0006
328	1	37	1	36	0	36	1	35	3831.9493	3831.94962	-0.0003
329	1	38	2	37	0	37	2	36	3831.9706	3831.97147	-0.0009
330	1	44	7	37	0	43	7	36	3831.9942	3831.99362	0.0006
331	1	46	8	38	0	45	8	37	3832.0013	3832.00112	0.0002
332	1	38	2	36	0	37	2	35	3832.079	3832.07877	0.0002
333	1	39	3	37	0	38	3	36	3832.0906	3832.09114	-0.0005
334	1	39	3	36	0	38	3	35	3832.0996	3832.10029	-0.0007
335	1	40	4	36	0	39	4	35	3832.1059	3832.10508	0.0008

336	1	38	1	37	0	37	1	36	3832.2213	3832.22144	-0.0001
337	1	39	2	38	0	38	2	37	3832.2407	3832.23989	0.0008
338	1	45	7	38	0	44	7	37	3832.2685	3832.26828	0.0002
339	1	42	5	37	0	41	5	36	3832.3186	3832.31926	-0.0007
340	1	39	2	37	0	38	2	36	3832.3556	3832.35579	-0.0002
341	1	40	3	38	0	39	3	37	3832.362	3832.36284	-0.0008
342	1	40	3	37	0	39	3	36	3832.3725	3832.37331	-0.0008
343	1	40	1	40	0	39	1	39	3832.446	3832.44523	0.0008
344	1	39	1	38	0	38	1	37	3832.4946	3832.49371	0.0009
345	1	40	2	39	0	39	2	38	3832.5088	3832.50882	0
346	1	46	7	39	0	45	7	38	3832.5445	3832.54355	0.001
347	1	41	3	39	0	40	3	38	3832.6351	3832.63519	-0.0001
348	1	41	3	38	0	40	3	37	3832.647	3832.64711	-0.0001
349	1	41	1	41	0	40	1	40	3832.7079	3832.7087	-0.0008
350	1	41	2	40	0	40	2	39	3832.7785	3832.77825	0.0002
351	1	42	3	40	0	41	3	39	3832.9082	3832.90816	0
352	1	42	3	39	0	41	3	38	3832.9223	3832.92171	0.0006
353	1	43	4	39	0	42	4	38	3832.9241	3832.92435	-0.0003
354	1	42	2	40	0	41	2	39	3833.192	3833.19194	0.0001
355	1	43	3	40	0	42	3	39	3833.1973	3833.1971	0.0002
356	1	44	4	40	0	43	4	39	3833.1993	3833.19877	0.0005
357	1	43	2	42	0	42	2	41	3833.3196	3833.31857	0.001
358	1	44	3	42	0	43	3	41	3833.4569	3833.45598	0.0009
359	1	43	2	41	0	42	2	40	3833.4719	3833.47229	-0.0004
360	1	44	3	41	0	43	3	40	3833.4733	3833.47329	0
361	1	45	4	41	0	44	4	40	3833.4736	3833.47386	-0.0003
362	1	44	2	43	0	43	2	42	3833.5894	3833.58945	0
363	1	46	4	42	0	45	4	41	3833.75	3833.74961	0.0004
364	1	45	3	42	0	44	3	41	3833.7501	3833.75028	-0.0002
365	1	45	2	44	0	44	2	43	3833.8603	3833.86079	-0.0005
366	1	46	3	43	0	45	3	42	3834.0278	3834.02809	-0.0003
367	1	45	2	43	0	44	2	42	3834.035	3834.0353	-0.0003
368	1	46	2	45	0	45	2	44	3834.1336	3834.13259	0.001
369	1	47	3	45	0	46	3	44	3834.2825	3834.28227	0.0002
370	1	47	1	47	0	46	1	46	3834.2988	3834.29838	0.0004
371	1	47	3	44	0	46	3	43	3834.3061	3834.30672	-0.0006
372	1	46	2	44	0	45	2	43	3834.3186	3834.31792	0.0007
373	1	47	2	46	0	46	2	45	3834.4043	3834.40483	-0.0005
374	1	47	1	46	0	46	1	45	3834.6864	3834.68615	0.0003
375	1	54	6	48	0	53	6	47	3835.2386	3835.23937	-0.0008
376	1	55	6	49	0	54	6	48	3835.5203	3835.52003	0.0003
377	1	54	4	51	0	53	4	50	3835.9764	3835.97636	0
378	1	54	4	50	0	53	4	49	3835.979	3835.97917	-0.0002
379	1	55	4	52	0	54	4	51	3836.2573	3836.25758	-0.0003
380	1	55	4	51	0	54	4	50	3836.2608	3836.2608	0

381	1	58	6	52	0	57	6	51	3836.365	3836.36545	-0.0005
382	1	56	4	53	0	55	4	52	3836.5389	3836.5394	-0.0005
383	1	56	4	52	0	55	4	51	3836.5437	3836.54306	0.0006
384	1	59	6	53	0	58	6	52	3836.6475	3836.64839	-0.0009
385	1	57	4	53	0	56	4	52	3836.8263	3836.82598	0.0003
386	1	58	4	55	0	57	4	54	3837.1052	3837.1048	0.0004
387	1	58	4	54	0	57	4	53	3837.1093	3837.10954	-0.0002
388	1	62	6	56	0	61	6	55	3837.5009	3837.50055	0.0003

B.8  $^{79}\text{BrNO } 3\nu_1 + \nu_3$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu'$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	59	8	51	0	60	8	52	3549.331	3549.33135	-0.00035
2	1	58	8	50	0	59	8	51	3549.462	3549.46264	-0.00064
3	1	58	7	51	0	59	7	52	3550.249	3550.24932	-0.00032
4	1	51	8	43	0	52	8	44	3550.428	3550.42824	-0.00024
5	1	50	8	42	0	51	8	43	3550.574	3550.57366	0.000345
6	1	55	7	48	0	56	7	49	3550.651	3550.65093	0.000067
7	1	68	4	64	0	69	4	65	3550.789	3550.78859	0.000406
8	1	54	7	47	0	55	7	48	3550.789	3550.78859	0.000412
9	1	53	7	46	0	54	7	47	3550.929	3550.92935	-0.00035
10	1	53	7	46	0	54	7	47	3550.929	3550.92933	-0.00033
11	1	58	6	52	0	59	6	53	3550.933	3550.93335	-0.00035
12	1	47	8	39	0	48	8	40	3551.023	3551.02242	0.000583
13	1	65	4	62	0	66	4	63	3551.126	3551.12572	0.000283
14	1	65	4	61	0	66	4	62	3551.129	3551.12873	0.000266
15	1	46	8	38	0	47	8	39	3551.177	3551.17727	-0.00027
16	1	50	7	43	0	51	7	44	3551.36	3551.3604	-0.0004
17	1	69	1	68	0	70	1	69	3551.406	3551.40644	-0.00044
18	1	69	0	69	0	70	0	70	3551.432	3551.43178	0.000221
19	1	54	6	48	0	55	6	49	3551.473	3551.47343	-0.00043
20	1	62	4	58	0	63	4	59	3551.487	3551.48726	-0.00026
21	1	49	7	42	0	50	7	43	3551.508	3551.5074	0.0006
22	1	67	2	65	0	68	2	66	3551.565	3551.5649	0.000097
23	1	67	1	67	0	68	1	68	3551.65	3551.64959	0.000413
24	1	66	2	64	0	67	2	65	3551.677	3551.67712	-0.00012
25	1	60	4	57	0	61	4	58	3551.735	3551.73545	-0.00045
26	1	66	1	66	0	67	1	67	3551.769	3551.76916	-0.00016
27	1	66	0	66	0	67	0	67	3551.787	3551.78698	0.000024
28	1	59	4	55	0	60	4	56	3551.864	3551.86353	0.000475
29	1	65	1	65	0	66	1	66	3551.891	3551.89073	0.000273
30	1	58	4	54	0	59	4	55	3551.993	3551.99274	0.000263
31	1	60	3	57	0	61	3	58	3552.119	3552.11955	-0.00055
32	1	57	4	53	0	58	4	54	3552.124	3552.12464	-0.00064

33	1	40	8	32	0	41	8	33	3552.14	3552.14048	-0.00048
34	1	53	5	48	0	54	5	49	3552.194	3552.19432	-0.00032
35	1	61	2	60	0	62	2	61	3552.227	3552.22637	0.000634
36	1	62	1	61	0	63	1	62	3552.238	3552.23853	-0.00053
37	1	61	0	61	0	62	0	62	3552.413	3552.4129	0.000096
38	1	60	1	59	0	61	1	60	3552.491	3552.49152	-0.00052
39	1	59	2	57	0	60	2	58	3552.515	3552.51562	-0.00062
40	1	60	1	60	0	61	1	61	3552.524	3552.5238	0.000201
41	1	58	2	57	0	59	2	58	3552.616	3552.61587	0.00013
42	1	50	5	45	0	51	5	46	3552.624	3552.62375	0.000247
43	1	56	3	53	0	57	3	54	3552.636	3552.63652	-0.00052
44	1	53	4	49	0	54	4	50	3552.67	3552.66993	0.000068
45	1	55	3	53	0	56	3	54	3552.763	3552.76254	0.000457
46	1	55	3	52	0	56	3	53	3552.77	3552.77042	-0.00042
47	1	57	2	55	0	58	2	56	3552.772	3552.77247	-0.00047
48	1	49	5	44	0	50	5	45	3552.772	3552.77216	-0.00016
49	1	58	0	58	0	59	0	59	3552.811	3552.81108	-8.4E-05
50	1	56	2	55	0	57	2	56	3552.885	3552.88444	0.000564
51	1	53	3	50	0	54	3	51	3553.045	3553.04514	-0.00014
52	1	47	5	42	0	48	5	43	3553.073	3553.07278	0.000221
53	1	56	0	56	0	57	0	57	3553.084	3553.0839	0.000101
54	1	50	4	46	0	51	4	47	3553.101	3553.10034	0.000664
55	1	46	5	41	0	47	5	42	3553.227	3553.22658	0.000425
56	1	54	1	53	0	55	1	54	3553.293	3553.29248	0.000519
57	1	54	1	54	0	55	1	55	3553.342	3553.34235	-0.00035
58	1	48	4	44	0	49	4	45	3553.398	3553.39821	-0.00021
59	1	52	2	50	0	53	2	51	3553.451	3553.45151	-0.00051
60	1	52	1	52	0	53	1	53	3553.629	3553.62936	-0.00036
61	1	46	4	42	0	47	4	43	3553.702	3553.70233	-0.00033
62	1	50	2	49	0	51	2	50	3553.735	3553.73527	-0.00027
63	1	49	2	47	0	50	2	48	3553.883	3553.88325	-0.00025
64	1	47	3	45	0	48	3	46	3553.919	3553.91928	-0.00028
65	1	41	5	36	0	42	5	37	3554.024	3554.02447	-0.00047
66	1	48	2	46	0	49	2	47	3554.031	3554.03134	-0.00034
67	1	47	2	46	0	48	2	47	3554.186	3554.18622	-0.00022
68	1	40	5	35	0	41	5	36	3554.189	3554.18952	-0.00052
69	1	48	1	48	0	49	1	49	3554.225	3554.22513	-0.00013
70	1	45	3	42	0	46	3	43	3554.228	3554.2286	-0.0006
71	1	47	0	47	0	48	0	48	3554.403	3554.40287	0.000126
72	1	46	1	45	0	47	1	46	3554.465	3554.46454	0.000456
73	1	45	2	43	0	46	2	44	3554.487	3554.48695	0.000048
74	1	45	2	44	0	46	2	45	3554.496	3554.49554	0.000464
75	1	41	4	37	0	42	4	38	3554.499	3554.49963	-0.00063
76	1	34	6	28	0	35	6	29	3554.642	3554.64222	-0.00022
77	1	44	2	43	0	45	2	44	3554.654	3554.65453	-0.00053

78	1	45	1	45	0	46	1	46	3554.691	3554.69153	-0.00053
79	1	42	3	40	0	43	3	41	3554.706	3554.70534	0.00066
80	1	43	2	41	0	44	2	42	3554.802	3554.80196	0.00004
81	1	43	2	42	0	44	2	43	3554.813	3554.81276	0.000244
82	1	41	3	38	0	42	3	39	3554.869	3554.86839	0.000615
83	1	43	1	42	0	44	1	43	3554.936	3554.93658	-0.00058
84	1	42	2	41	0	43	2	42	3554.975	3554.97437	0.000633
85	1	41	2	40	0	42	2	41	3555.138	3555.13831	-0.00031
86	1	36	4	32	0	37	4	33	3555.345	3555.34442	0.00058
87	1	40	1	39	0	41	1	40	3555.424	3555.4236	0.000402
88	1	35	4	31	0	36	4	32	3555.52	3555.51942	0.000576
89	1	39	1	39	0	40	1	40	3555.672	3555.67135	0.000649
90	1	38	0	38	0	39	0	39	3555.865	3555.86453	0.000472
91	1	35	3	33	0	36	3	34	3555.89	3555.88974	0.000259
92	1	37	0	37	0	38	0	38	3556.037	3556.03647	0.00053
93	1	34	3	32	0	35	3	33	3556.067	3556.0669	0.000103
94	1	10	10	0	0	10	10	1	3558.835	3558.83443	0.000568
95	1	11	10	1	0	11	10	2	3558.856	3558.8564	-0.0004
96	1	11	9	2	0	11	9	3	3559.84	3559.84062	-0.00062
97	1	12	9	3	0	12	9	4	3559.862	3559.86188	0.000117
98	1	8	7	1	0	8	7	2	3561.451	3561.45089	0.000115
99	1	9	7	2	0	9	7	3	3561.468	3561.46741	0.000594
100	1	11	7	4	0	11	7	5	3561.508	3561.50838	-0.00038
101	1	8	6	2	0	8	6	3	3562.132	3562.13223	-0.00023
102	1	9	6	3	0	9	6	4	3562.149	3562.14871	0.00029
103	1	6	5	1	0	6	5	2	3562.682	3562.68186	0.000142
104	1	5	4	1	0	5	4	2	3563.145	3563.14489	0.000108
105	1	14	4	10	0	13	4	9	3566.74	3566.73959	0.000415
106	1	15	4	11	0	14	4	10	3567.013	3567.01255	0.000451
107	1	15	3	12	0	14	3	11	3567.383	3567.38357	-0.00057
108	1	17	4	13	0	16	4	12	3567.565	3567.56522	-0.00022
109	1	16	3	13	0	15	3	12	3567.658	3567.65747	0.000526
110	1	18	4	14	0	17	4	13	3567.844	3567.84388	0.000119
111	1	15	0	15	0	14	0	14	3567.852	3567.85152	0.000482
112	1	17	0	17	0	16	0	16	3568.4	3568.39974	0.000262
113	1	18	2	17	0	17	2	16	3568.474	3568.47466	-0.00066
114	1	18	1	18	0	17	1	17	3568.57	3568.57051	-0.00051
115	1	21	4	17	0	20	4	16	3568.691	3568.69035	0.00065
116	1	20	2	19	0	19	2	18	3569.036	3569.03618	-0.00018
117	1	21	3	18	0	20	3	17	3569.061	3569.06065	0.000353
118	1	24	5	19	0	23	5	18	3569.08	3569.08063	-0.00063
119	1	20	1	19	0	19	1	18	3569.264	3569.26431	-0.00031
120	1	21	1	21	0	20	1	20	3569.401	3569.40046	0.000538
121	1	32	8	24	0	31	8	23	3569.424	3569.42389	0.000108
122	1	22	2	21	0	21	2	20	3569.605	3569.60559	-0.00059

123	1	25	4	21	0	24	4	20	3569.846	3569.84644	-0.00044
124	1	27	5	22	0	26	5	21	3569.961	3569.9606	0.000401
125	1	24	2	23	0	23	2	22	3570.181	3570.18066	0.000337
126	1	32	7	25	0	31	7	24	3570.207	3570.20656	0.000436
127	1	28	5	23	0	27	5	22	3570.258	3570.25796	0.000044
128	1	25	2	24	0	24	2	23	3570.472	3570.47139	0.000611
129	1	25	2	23	0	24	2	22	3570.503	3570.50246	0.000539
130	1	25	1	25	0	24	1	24	3570.534	3570.53347	0.00053
131	1	36	8	28	0	35	8	27	3570.66	3570.66033	-0.00033
132	1	25	1	24	0	24	1	23	3570.721	3570.72085	0.000147
133	1	26	2	24	0	25	2	23	3570.8	3570.79989	0.000109
134	1	37	8	29	0	36	8	28	3570.974	3570.97441	-0.00041
135	1	28	3	25	0	27	3	24	3571.105	3571.10498	0.000019
136	1	38	8	30	0	37	8	29	3571.289	3571.2888	0.000199
137	1	34	6	28	0	33	6	27	3571.501	3571.50089	0.000107
138	1	30	3	27	0	29	3	26	3571.706	3571.70646	-0.00046
139	1	29	1	28	0	28	1	27	3571.919	3571.91927	-0.00027
140	1	30	1	30	0	29	1	29	3571.987	3571.98671	0.000286
141	1	34	5	29	0	33	5	28	3572.079	3572.07886	0.000138
142	1	30	0	30	0	29	0	29	3572.116	3572.11667	-0.00067
143	1	41	8	33	0	40	8	32	3572.245	3572.2454	-0.0004
144	1	33	1	33	0	32	1	32	3572.879	3572.87865	0.000354
145	1	37	5	32	0	36	5	31	3573.015	3573.0149	0.000098
146	1	34	2	33	0	33	2	32	3573.166	3573.16592	0.000085
147	1	35	3	32	0	34	3	31	3573.242	3573.24257	-0.00057
148	1	35	2	34	0	34	2	33	3573.474	3573.4737	0.000305
149	1	38	4	34	0	37	4	33	3573.807	3573.8069	0.000104
150	1	37	3	35	0	36	3	34	3573.863	3573.86327	-0.00027
151	1	39	4	35	0	38	4	34	3574.124	3574.1235	0.000499
152	1	47	8	39	0	46	8	38	3574.206	3574.20544	0.000564
153	1	45	7	38	0	44	7	37	3574.328	3574.32763	0.000374
154	1	42	5	37	0	41	5	36	3574.61	3574.60937	0.000627
155	1	38	1	37	0	37	1	36	3574.713	3574.71345	-0.00045
156	1	39	2	37	0	38	2	36	3574.85	3574.85009	-8.8E-05
157	1	40	1	40	0	39	1	39	3575.015	3575.0153	-0.0003
158	1	40	0	40	0	39	0	39	3575.138	3575.1386	-0.0006
159	1	41	2	39	0	40	2	38	3575.504	3575.50465	-0.00065
160	1	45	4	41	0	44	4	40	3576.068	3576.06855	-0.00055
161	1	44	1	44	0	43	1	43	3576.271	3576.27167	-0.00067
162	1	45	3	42	0	44	3	41	3576.461	3576.46115	-0.00015
163	1	45	1	45	0	44	1	44	3576.589	3576.58948	-0.00048
164	1	46	3	43	0	45	3	42	3576.793	3576.79347	-0.00047
165	1	45	2	43	0	44	2	42	3576.837	3576.83729	-0.00029
166	1	46	2	44	0	45	2	43	3577.175	3577.17466	0.000336
167	1	47	1	47	0	46	1	46	3577.229	3577.22838	0.000622

168	1	47	2	46	0	46	2	45	3577.298	3577.29826	-0.00026
169	1	46	1	45	0	45	1	44	3577.306	3577.30554	0.000458
170	1	52	6	46	0	51	6	45	3577.353	3577.35294	0.000065
171	1	48	0	48	0	47	0	47	3577.656	3577.65619	-0.00019
172	1	49	3	46	0	48	3	45	3577.804	3577.80461	-0.00061
173	1	50	3	47	0	49	3	46	3578.144	3578.14371	0.000294
174	1	58	6	52	0	57	6	51	3579.43	3579.42998	0.00002
175	1	58	4	54	0	57	4	53	3580.503	3580.50308	-7.9E-05

B.9  $^{81}\text{BrNO } 3\nu_1 + \nu_3$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu''$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	61	6	55	0	62	6	56	3550.6137	3550.61371	0.00001
2	1	57	6	51	0	58	6	52	3551.124	3551.12441	0.00041
3	1	45	8	37	0	46	8	38	3551.3792	3551.37955	0.00035
4	1	56	4	52	0	57	4	53	3552.3174	3552.31724	-0.00016
5	1	43	7	36	0	44	7	37	3552.4803	3552.48066	0.00036
6	1	38	8	30	0	39	8	31	3552.5139	3552.51372	-0.00018
7	1	54	4	51	0	55	4	52	3552.5867	3552.58621	-0.0005
8	1	37	8	29	0	38	8	30	3552.6856	3552.68604	0.00044
9	1	53	4	50	0	54	4	51	3552.7259	3552.72561	-0.00029
10	1	41	7	34	0	42	7	35	3552.802	3552.80207	0.00006
11	1	36	8	28	0	37	8	29	3552.8571	3552.85749	0.00039
12	1	51	4	47	0	52	4	48	3553.0079	3553.00824	0.00034
13	1	35	8	27	0	36	8	28	3553.0316	3553.03158	-0.00002
14	1	50	4	46	0	51	4	47	3553.1535	3553.1537	0.0002
15	1	48	4	44	0	49	4	45	3553.4477	3553.44774	0.00004
16	1	50	3	48	0	51	3	49	3553.5238	3553.52412	0.00032
17	1	50	3	47	0	51	3	48	3553.526	3553.52597	-0.00003
18	1	32	8	24	0	33	8	25	3553.5643	3553.56409	-0.00021
19	1	49	3	47	0	50	3	48	3553.6697	3553.66959	-0.00011
20	1	49	3	46	0	50	3	47	3553.6723	3553.67214	-0.00016
21	1	30	8	22	0	31	8	23	3553.9298	3553.92935	-0.00046
22	1	34	7	27	0	35	7	28	3553.9931	3553.99322	0.00012
23	1	46	3	44	0	47	3	45	3554.1207	3554.12048	-0.00022
24	1	46	3	43	0	47	3	44	3554.1214	3554.12103	-0.00037
25	1	36	6	30	0	37	6	31	3554.3255	3554.3257	0.0002
26	1	42	4	38	0	43	4	39	3554.3797	3554.3796	-0.0001
27	1	45	2	43	0	46	2	44	3554.5347	3554.53509	0.00039
28	1	41	4	37	0	42	4	38	3554.5413	3554.54083	-0.00047
29	1	38	5	33	0	39	5	34	3554.5636	3554.56347	-0.00013
30	1	43	3	40	0	44	3	41	3554.5885	3554.58866	0.00016
31	1	42	3	39	0	43	3	40	3554.7482	3554.74828	0.00008
32	1	44	1	43	0	45	1	44	3554.8231	3554.82322	0.00012



33	1	39	4	35	0	40	4	36	3554.871	3554.87123	0.00023
34	1	36	5	31	0	37	5	32	3554.9057	3554.90596	0.00026
35	1	43	1	43	0	44	1	44	3555.0538	3555.05363	-0.00017
36	1	35	5	30	0	36	5	31	3555.0794	3555.07955	0.00015
37	1	39	3	37	0	40	3	38	3555.2402	3555.24003	-0.00017
38	1	38	3	35	0	39	3	36	3555.4083	3555.40811	-0.00019
39	1	40	1	39	0	41	1	40	3555.4659	3555.46571	-0.00019
40	1	39	2	38	0	40	2	39	3555.5104	3555.50996	-0.00044
41	1	35	4	31	0	36	4	32	3555.5535	3555.55316	-0.00034
42	1	37	3	34	0	38	3	35	3555.5791	3555.57906	-0.00004
43	1	38	2	37	0	39	2	38	3555.6784	3555.6786	0.0002
44	1	39	0	39	0	40	0	40	3555.7351	3555.73477	-0.00033
45	1	38	0	38	0	39	0	39	3555.9039	3555.90429	0.00039
46	1	30	5	25	0	31	5	26	3555.978	3555.97827	0.00027
47	1	37	0	37	0	38	0	38	3556.0733	3556.07374	0.00044
48	1	34	3	31	0	35	3	32	3556.0987	3556.09897	0.00027
49	1	35	2	34	0	36	2	35	3556.1941	3556.19361	-0.00049
50	1	34	2	32	0	35	2	33	3556.3537	3556.35377	0.00007
51	1	35	0	35	0	36	0	36	3556.4188	3556.41904	0.00024
52	1	34	1	33	0	35	1	34	3556.4885	3556.48814	-0.00036
53	1	34	1	34	0	35	1	35	3556.573	3556.57299	-0.00001
54	1	32	2	31	0	33	2	32	3556.7263	3556.72595	-0.00035
55	1	33	1	33	0	34	1	34	3556.7505	3556.75089	0.00039
56	1	33	0	33	0	34	0	34	3556.7725	3556.77212	-0.00038
57	1	31	2	30	0	32	2	31	3556.9088	3556.90861	-0.00019
58	1	32	1	32	0	33	1	33	3556.9299	3556.92942	-0.00048
59	1	31	1	31	0	32	1	32	3557.1118	3557.1118	0
60	1	26	4	22	0	27	4	23	3557.2053	3557.20578	0.00048
61	1	29	2	27	0	30	2	28	3557.2645	3557.26458	0.00008
62	1	29	2	28	0	30	2	29	3557.2766	3557.27621	-0.00039
63	1	30	1	30	0	31	1	31	3557.2941	3557.29421	0.00011
64	1	29	1	28	0	30	1	29	3557.3944	3557.39471	0.00031
65	1	28	2	26	0	29	2	27	3557.452	3557.45173	-0.00027
66	1	28	2	27	0	29	2	28	3557.4632	3557.46319	-0.00001
67	1	29	1	29	0	30	1	30	3557.4793	3557.47882	-0.00048
68	1	26	3	23	0	27	3	24	3557.5755	3557.576	0.0005
69	1	24	4	20	0	25	4	21	3557.5946	3557.59473	0.00013
70	1	27	2	25	0	28	2	26	3557.6414	3557.64113	-0.00027
71	1	27	1	26	0	28	1	27	3557.7716	3557.77118	-0.00042
72	1	12	11	1	0	12	11	2	3557.7756	3557.77565	0.00005
73	1	23	4	19	0	24	4	20	3557.7919	3557.79188	-0.00002
74	1	27	1	27	0	28	1	28	3557.8553	3557.85521	-0.00009
75	1	27	0	27	0	28	0	28	3557.8752	3557.87481	-0.00039
76	1	16	11	5	0	16	11	6	3557.8856	3557.88516	-0.00044
77	1	18	11	7	0	18	11	8	3557.9512	3557.95099	-0.00022

78	1	24	3	21	0	25	3	22	3557.964	3557.9636	-0.00041
79	1	25	2	24	0	26	2	25	3558.0379	3558.03796	0.00006
80	1	26	0	26	0	27	0	27	3558.0663	3558.06642	0.00012
81	1	25	1	24	0	26	1	25	3558.1564	3558.15644	0.00004
82	1	24	2	23	0	25	2	24	3558.2316	3558.23138	-0.00022
83	1	25	1	25	0	26	1	26	3558.2383	3558.23815	-0.00015
84	1	22	3	19	0	23	3	20	3558.3602	3558.3598	-0.0004
85	1	24	1	24	0	25	1	25	3558.4331	3558.43347	0.00037
86	1	24	0	24	0	25	0	25	3558.4519	3558.45148	-0.00042
87	1	18	4	14	0	19	4	15	3558.8063	3558.80597	-0.00033
88	1	10	10	0	0	10	10	1	3558.8151	3558.81541	0.00031
89	1	11	10	1	0	11	10	2	3558.8362	3558.83591	-0.00029
90	1	21	1	20	0	22	1	21	3558.9507	3558.95051	-0.00019
91	1	19	3	16	0	20	3	17	3558.9688	3558.96891	0.00011
92	1	21	1	21	0	22	1	22	3559.027	3559.02692	-0.00008
93	1	20	2	19	0	21	2	20	3559.0309	3559.03099	0.00009
94	1	20	1	19	0	21	1	20	3559.1538	3559.15331	-0.0005
95	1	20	1	20	0	21	1	21	3559.2286	3559.2281	-0.0005
96	1	19	2	18	0	20	2	19	3559.2372	3559.23693	-0.00027
97	1	14	4	10	0	15	4	11	3559.6522	3559.65223	0.00003
98	1	17	0	17	0	18	0	18	3559.8667	3559.86702	0.00032
99	1	16	1	16	0	17	1	17	3560.0539	3560.05411	0.00021
100	1	10	4	6	0	11	4	7	3560.5306	3560.531	0.0004
101	1	9	8	1	0	9	8	2	3560.6652	3560.6655	0.0003
102	1	13	8	5	0	13	8	6	3560.7534	3560.75338	-0.00002
103	1	11	7	4	0	11	7	5	3561.4897	3561.48993	0.00023
104	1	9	6	3	0	9	6	4	3562.1306	3562.13043	-0.00017
105	1	16	6	10	0	16	6	11	3562.3043	3562.30406	-0.00024
106	1	17	6	11	0	17	6	12	3562.335	3562.33484	-0.00016
107	1	7	4	3	0	7	4	4	3563.153	3563.1532	0.0002
108	1	8	5	3	0	7	5	2	3564.6371	3564.63734	0.00024
109	1	8	4	4	0	7	4	3	3565.1115	3565.11121	-0.00029
110	1	7	2	6	0	6	2	5	3565.4879	3565.48774	-0.00016
111	1	10	4	6	0	9	4	5	3565.6342	3565.63403	-0.00017
112	1	12	5	7	0	11	5	6	3565.6894	3565.68893	-0.00047
113	1	11	4	7	0	10	4	6	3565.8984	3565.89793	-0.00047
114	1	8	1	7	0	7	1	6	3565.9277	3565.92804	0.00034
115	1	13	5	8	0	12	5	7	3565.9559	3565.95588	-0.00003
116	1	14	5	9	0	13	5	8	3566.2265	3566.22658	0.00008
117	1	10	2	9	0	9	2	8	3566.267	3566.26665	-0.00036
118	1	15	5	10	0	14	5	9	3566.497	3566.49664	-0.00036
119	1	12	3	9	0	11	3	8	3566.5337	3566.53405	0.00035
120	1	11	1	10	0	10	1	9	3566.7242	3566.72376	-0.00044
121	1	14	1	14	0	13	1	13	3567.4462	3567.44594	-0.00026
122	1	16	3	13	0	15	3	12	3567.6148	3567.6149	0.0001

123	1	36	6	30	0	35	6	29	3572.0444	3572.04431	-0.0001
124	1	43	3	41	0	42	3	40	3575.691	3575.69141	0.00041
125	1	50	7	43	0	49	7	42	3575.8873	3575.88701	-0.00029
126	1	44	3	42	0	43	3	41	3576.0163	3576.01629	-0.00001
127	1	44	3	41	0	43	3	40	3576.0357	3576.0362	0.0005
128	1	53	8	45	0	52	8	44	3576.1175	3576.11754	0.00004
129	1	47	5	42	0	46	5	41	3576.1494	3576.14906	-0.00034
130	1	46	3	43	0	45	3	42	3576.695	3576.69527	0.00027
131	1	55	8	47	0	54	8	46	3576.8028	3576.80279	-0.00001
132	1	53	7	46	0	52	7	45	3576.8998	3576.90005	0.00025
133	1	56	8	48	0	55	8	47	3577.1464	3577.14597	-0.00043
134	1	51	5	46	0	50	5	45	3577.4855	3577.48509	-0.00041
135	1	53	6	47	0	52	6	46	3577.5824	3577.58219	-0.00021
136	1	48	2	46	0	47	2	45	3577.7513	3577.75118	-0.00012
137	1	56	7	49	0	55	7	48	3577.9302	3577.92994	-0.00026
138	1	51	4	48	0	50	4	47	3577.9668	3577.96663	-0.00017
139	1	59	8	51	0	58	8	50	3578.1911	3578.19095	-0.00015
140	1	49	1	48	0	48	1	47	3578.198	3578.19844	0.00044
141	1	52	4	49	0	51	4	48	3578.3054	3578.30498	-0.00042
142	1	51	2	50	0	50	2	49	3578.5168	3578.51638	-0.00042
143	1	60	8	52	0	59	8	51	3578.5436	3578.5441	0.0005
144	1	53	4	49	0	52	4	48	3578.6475	3578.64778	0.00028
145	1	52	2	51	0	51	2	50	3578.851	3578.85053	-0.00047
146	1	54	4	50	0	53	4	49	3578.9904	3578.99068	0.00028
147	1	53	2	52	0	52	2	51	3579.1854	3579.18519	-0.00021
148	1	62	8	54	0	61	8	53	3579.2507	3579.25063	-0.00007
149	1	60	7	53	0	59	7	52	3579.3262	3579.32608	-0.00012
150	1	55	4	52	0	54	4	51	3579.3323	3579.33199	-0.00031
151	1	56	4	53	0	55	4	52	3579.6782	3579.67777	-0.00043
152	1	64	8	56	0	63	8	55	3579.9669	3579.9674	0.0005
153	1	57	4	53	0	56	4	52	3580.0299	3580.02987	-0.00003
154	1	62	7	55	0	61	7	54	3580.0357	3580.03594	0.00024
155	1	56	3	54	0	55	3	53	3580.0438	3580.04348	-0.00032
156	1	56	2	55	0	55	2	54	3580.1998	3580.1998	0
157	1	57	3	55	0	56	3	54	3580.3901	3580.3906	0.0005
158	1	56	2	54	0	55	2	53	3580.5305	3580.53043	-0.00007
159	1	56	1	55	0	55	1	54	3580.5561	3580.5561	0
160	1	59	4	56	0	58	4	55	3580.7264	3580.72628	-0.00012
161	1	58	1	58	0	57	1	57	3580.7401	3580.74041	0.00031
162	1	57	1	56	0	56	1	55	3580.8973	3580.89687	-0.00043
163	1	60	4	56	0	59	4	55	3581.0859	3581.08638	0.00048
164	1	59	3	57	0	58	3	56	3581.0895	3581.0899	0.0004
165	1	60	3	58	0	59	3	57	3581.4404	3581.44008	-0.00032
166	1	60	3	57	0	59	3	56	3581.5363	3581.53662	0.00032
167	1	60	2	59	0	59	2	58	3581.5727	3581.57312	0.00042

168	1	62	4	59	0	61	4	58	3581.7891	3581.78911	0.00001
169	1	63	4	59	0	62	4	58	3582.1573	3582.15687	-0.00043
170	1	62	2	61	0	61	2	60	3582.2666	3582.26639	-0.00021
171	1	64	4	60	0	63	4	59	3582.5192	3582.51949	0.00029
172	1	62	1	61	0	61	1	60	3582.6233	3582.62301	-0.00029
173	1	65	4	62	0	64	4	61	3582.8687	3582.86877	0.00007
174	1	65	4	61	0	64	4	60	3582.8818	3582.88145	-0.00035
175	1	63	1	62	0	62	1	61	3582.972	3582.97159	-0.00041
176	1	63	2	61	0	62	2	60	3583.0483	3583.0481	-0.00021
177	1	65	1	65	0	64	1	64	3583.1306	3583.13097	0.00037
178	1	66	4	63	0	65	4	62	3583.2329	3583.23254	-0.00036
179	1	66	2	65	0	65	2	64	3583.6748	3583.67496	0.00016
180	1	66	2	64	0	65	2	63	3584.1505	3584.15021	-0.00029
181	1	68	1	68	0	67	1	67	3584.1762	3584.17618	-0.00003
182	1	69	1	69	0	68	1	68	3584.528	3584.52754	-0.00046
183	1	70	4	67	0	69	4	66	3584.7024	3584.70254	0.00014
184	1	68	1	67	0	67	1	66	3584.7311	3584.73099	-0.00011
185	1	70	1	70	0	69	1	69	3584.8802	3584.88003	-0.00017
186	1	68	2	66	0	67	2	65	3584.8911	3584.89067	-0.00043

B.10  $^{79}\text{BrNO } \nu_1 + \nu_2 - \nu_3$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu''$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	69	4	66	0	70	4	67	2046.8229	2046.82234	0.0006
2	1	68	0	68	0	69	0	69	2047.0975	2047.09733	0.0002
3	1	67	0	67	0	68	0	68	2047.2876	2047.28743	0.0002
4	1	66	4	62	0	67	4	63	2047.3719	2047.37146	0.0004
5	1	65	1	65	0	66	1	66	2047.6606	2047.66046	0.0001
6	1	64	0	64	0	65	0	65	2047.8618	2047.86179	0
7	1	63	1	62	0	64	1	63	2048.1072	2048.1071	0.0001
8	1	63	2	61	0	64	2	62	2048.1081	2048.10812	0
9	1	62	4	59	0	63	4	60	2048.1113	2048.11112	0.0002
10	1	62	1	62	0	63	1	63	2048.2388	2048.23878	0
11	1	62	0	62	0	63	0	63	2048.2481	2048.24808	0
12	1	62	2	60	0	63	2	61	2048.2919	2048.29193	0
13	1	62	1	61	0	63	1	62	2048.295	2048.29478	0.0002
14	1	61	3	59	0	62	3	60	2048.384	2048.38394	0.0001
15	1	61	1	61	0	62	1	62	2048.4328	2048.43296	-0.0002
16	1	61	0	61	0	62	0	62	2048.4422	2048.44224	0
17	1	58	7	51	0	59	7	52	2048.462	2048.46186	0.0001
18	1	56	8	48	0	57	8	49	2048.6638	2048.66409	-0.0003
19	1	59	2	57	0	60	2	58	2048.8493	2048.84944	-0.0001
20	1	58	4	55	0	59	4	56	2048.8688	2048.86862	0.0002

21	1	58	2	57	0	59	2	58	2049.0041	2049.0042	-0.0001
22	1	56	6	50	0	57	6	51	2049.0067	2049.00656	0.0001
23	1	57	4	54	0	58	4	55	2049.0606	2049.06038	0.0002
24	1	57	2	55	0	58	2	56	2049.226	2049.22624	-0.0002
25	1	54	7	47	0	55	7	48	2049.2364	2049.23642	0
26	1	53	7	46	0	54	7	47	2049.4324	2049.43237	0
27	1	52	7	45	0	53	7	46	2049.6293	2049.62925	0.0001
28	1	54	4	50	0	55	4	51	2049.6417	2049.64159	0.0001
29	1	53	5	48	0	54	5	49	2049.7264	2049.72617	0.0002
30	1	54	3	52	0	55	3	53	2049.7269	2049.72705	-0.0002
31	1	54	3	51	0	55	3	52	2049.7307	2049.73085	-0.0001
32	1	50	8	42	0	51	8	43	2049.8429	2049.84317	-0.0003
33	1	53	1	52	0	54	1	53	2050.0179	2050.01812	-0.0002
34	1	52	4	48	0	53	4	49	2050.0336	2050.03351	0.0001
35	1	51	2	49	0	52	2	50	2050.3815	2050.38174	-0.0002
36	1	50	4	46	0	51	4	47	2050.4292	2050.42924	0
37	1	50	0	50	0	51	0	51	2050.6219	2050.62237	-0.0005
38	1	46	8	38	0	47	8	39	2050.6474	2050.64757	-0.0002
39	1	49	3	46	0	50	3	47	2050.7145	2050.71461	-0.0001
40	1	48	4	44	0	49	4	45	2050.8287	2050.82874	0
41	1	45	8	37	0	46	8	38	2050.8509	2050.85095	0
42	1	47	3	45	0	48	3	46	2051.1154	2051.11542	0
43	1	46	3	43	0	47	3	44	2051.3167	2051.31697	-0.0003
44	1	46	2	45	0	47	2	46	2051.3804	2051.38066	-0.0003
45	1	45	2	43	0	46	2	44	2051.5752	2051.57558	-0.0004
46	1	44	4	40	0	45	4	41	2051.6389	2051.63898	-0.0001
47	1	43	3	41	0	44	3	42	2051.9289	2051.92914	-0.0002
48	1	42	5	37	0	43	5	38	2051.9403	2051.94024	0.0001
49	1	43	2	41	0	44	2	42	2051.9817	2051.98208	-0.0004
50	1	43	1	43	0	44	1	44	2052.0505	2052.05099	-0.0005
51	1	41	3	38	0	42	3	39	2052.3402	2052.34043	-0.0002
52	1	41	2	39	0	42	2	40	2052.3924	2052.39282	-0.0004
53	1	38	3	36	0	39	3	37	2052.9669	2052.96704	-0.0001
54	1	37	0	37	0	38	0	38	2053.3047	2053.30516	-0.0005
55	1	36	3	33	0	37	3	34	2053.3873	2053.38758	-0.0003
56	1	35	5	30	0	36	5	31	2053.407	2053.40695	0
57	1	34	6	28	0	35	6	29	2053.487	2053.48674	0.0003
58	1	32	6	26	0	33	6	27	2053.9159	2053.91583	0.0001
59	1	10	8	2	0	10	8	3	2061.2135	2061.21344	0.0001
60	1	7	7	0	0	7	7	1	2061.3705	2061.37017	0.0003
61	1	10	7	3	0	10	7	4	2061.3929	2061.39268	0.0002
62	1	10	6	4	0	10	6	5	2061.5486	2061.54836	0.0002
63	1	8	5	3	0	8	5	4	2061.6646	2061.66447	0.0001
64	1	11	5	6	0	11	5	7	2061.6895	2061.6895	0
65	1	6	4	2	0	6	4	3	2061.76	2061.76008	-0.0001

66	1	12	4	8	0	11	4	7	2064.7294	2064.72942	0
67	1	13	3	10	0	12	3	9	2065.0675	2065.06773	-0.0002
68	1	14	4	10	0	13	4	9	2065.2386	2065.2387	-0.0001
69	1	15	4	11	0	14	4	10	2065.4944	2065.49456	-0.0002
70	1	17	4	13	0	16	4	12	2066.0087	2066.00871	0
71	1	17	1	17	0	16	1	16	2066.1241	2066.12458	-0.0005
72	1	17	0	17	0	16	0	16	2066.1901	2066.1908	-0.0007
73	1	19	1	18	0	18	1	17	2066.7708	2066.77136	-0.0006
74	1	20	2	19	0	19	2	18	2066.9256	2066.92596	-0.0004
75	1	20	0	20	0	19	0	19	2066.9607	2066.96136	-0.0007
76	1	21	2	20	0	20	2	19	2067.1855	2067.186	-0.0005
77	1	21	1	20	0	20	1	19	2067.2989	2067.29965	-0.0008
78	1	23	1	22	0	22	1	21	2067.8306	2067.83112	-0.0005
79	1	24	4	20	0	23	4	19	2067.8333	2067.83356	-0.0003
80	1	24	0	24	0	23	0	23	2067.9951	2067.99581	-0.0007
81	1	27	5	22	0	26	5	21	2068.5194	2068.51935	0
82	1	27	2	25	0	26	2	24	2068.8003	2068.80076	-0.0005
83	1	27	1	26	0	26	1	25	2068.9027	2068.90321	-0.0005
84	1	28	1	27	0	27	1	26	2069.1725	2069.17308	-0.0006
85	1	29	2	28	0	28	2	27	2069.2916	2069.292	-0.0004
86	1	30	3	27	0	29	3	26	2069.5164	2069.51676	-0.0004
87	1	31	2	30	0	30	2	29	2069.8249	2069.82537	-0.0005
88	1	33	5	28	0	32	5	27	2070.1281	2070.12794	0.0002
89	1	33	3	30	0	32	3	29	2070.3267	2070.32701	-0.0003
90	1	33	2	31	0	32	2	30	2070.4357	2070.43624	-0.0005
91	1	35	6	29	0	34	6	28	2070.5386	2070.53845	0.0002
92	1	37	8	29	0	36	8	28	2070.7509	2070.75091	0
93	1	36	4	32	0	35	4	31	2071.0522	2071.05231	-0.0001
94	1	37	0	37	0	36	0	36	2071.4004	2071.40091	-0.0005
95	1	38	1	38	0	37	1	37	2071.5651	2071.56559	-0.0005
96	1	40	8	32	0	39	8	31	2071.574	2071.57413	-0.0001
97	1	40	1	40	0	39	1	39	2072.0957	2072.09626	-0.0006
98	1	42	7	35	0	41	7	34	2072.3047	2072.30456	0.0001
99	1	42	1	42	0	41	1	41	2072.6284	2072.6289	-0.0005
100	1	42	3	39	0	41	3	38	2072.8046	2072.80493	-0.0003
101	1	42	2	40	0	41	2	39	2072.9599	2072.96047	-0.0006
102	1	45	8	37	0	44	8	36	2072.9606	2072.96072	-0.0001
103	1	44	1	44	0	43	1	43	2073.1631	2073.16345	-0.0004
104	1	44	2	43	0	43	2	42	2073.3533	2073.35365	-0.0003
105	1	45	1	45	0	44	1	44	2073.4311	2073.43144	-0.0003
106	1	45	0	45	0	44	0	44	2073.5226	2073.52301	-0.0004
107	1	47	7	40	0	46	7	39	2073.6987	2073.69853	0.0002
108	1	47	4	43	0	46	4	42	2074.1018	2074.10169	0.0001
109	1	49	3	46	0	48	3	45	2074.7833	2074.78344	-0.0001

B.11  $^{81}\text{BrNO } \nu_1 + \nu_2 - \nu_3$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu'$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	68	1	68	0	69	1	69	2047.2102	2047.20966	0.0005
2	1	68	1	67	0	69	1	68	2047.2404	2047.24037	0
3	1	67	0	67	0	68	0	68	2047.4028	2047.40312	-0.0003
4	1	66	1	66	0	67	1	67	2047.5856	2047.58611	-0.0005
5	1	66	0	66	0	67	0	67	2047.5912	2047.59166	-0.0005
6	1	63	7	56	0	64	7	57	2047.6145	2047.61427	0.0002
7	1	65	1	65	0	66	1	66	2047.7758	2047.77535	0.0004
8	1	65	0	65	0	66	0	66	2047.7808	2047.78085	-0.0001
9	1	65	1	64	0	66	1	65	2047.7929	2047.7926	0.0003
10	1	62	7	55	0	63	7	56	2047.8013	2047.80118	0.0001
11	1	61	8	53	0	62	8	54	2047.8185	2047.81818	0.0003
12	1	61	8	53	0	62	8	54	2047.819	2047.81818	0.0008
13	1	63	4	60	0	64	4	61	2047.9967	2047.99647	0.0002
14	1	63	4	59	0	64	4	60	2047.997	2047.9971	-0.0001
15	1	61	6	55	0	62	6	56	2048.1383	2048.13831	0
16	1	63	2	61	0	64	2	62	2048.1476	2048.14805	-0.0005
17	1	60	4	57	0	61	4	58	2048.5586	2048.55931	-0.0007
18	1	60	4	56	0	61	4	57	2048.56	2048.5596	0.0004
19	1	57	8	49	0	58	8	50	2048.5781	2048.57796	0.0001
20	1	60	1	59	0	61	1	60	2048.7269	2048.72695	-0.0001
21	1	56	8	48	0	57	8	49	2048.7703	2048.77008	0.0002
22	1	59	1	59	0	60	1	60	2048.9249	2048.92522	-0.0003
23	1	56	7	49	0	57	7	50	2048.9407	2048.94093	-0.0002
24	1	58	0	58	0	59	0	59	2049.1231	2049.12367	-0.0006
25	1	54	8	46	0	55	8	47	2049.1565	2049.15695	-0.0005
26	1	57	3	54	0	58	3	55	2049.2127	2049.21259	0.0001
27	1	57	0	57	0	58	0	58	2049.3188	2049.31815	0.0007
28	1	53	8	45	0	54	8	46	2049.3512	2049.3517	-0.0005
29	1	55	4	51	0	56	4	52	2049.5155	2049.51508	0.0004
30	1	54	5	49	0	55	5	50	2049.6042	2049.60434	-0.0001
31	1	54	4	50	0	55	4	51	2049.7081	2049.70886	-0.0008
32	1	54	2	52	0	55	2	53	2049.8428	2049.84331	-0.0005
33	1	53	4	49	0	54	4	50	2049.903	2049.90355	-0.0005
34	1	54	1	54	0	55	1	55	2049.9032	2049.90265	0.0006
35	1	54	0	54	0	55	0	55	2049.9054	2049.90558	-0.0002
36	1	50	7	43	0	51	7	44	2050.1128	2050.11218	0.0006
37	1	49	8	41	0	50	8	42	2050.1394	2050.1395	-0.0001
38	1	52	1	52	0	53	1	53	2050.2991	2050.29861	0.0005
39	1	51	1	50	0	52	1	51	2050.4574	2050.45681	0.0006
40	1	50	4	46	0	51	4	47	2050.4926	2050.49296	-0.0004
41	1	51	0	51	0	52	0	52	2050.4994	2050.49907	0.0003

42	1	50	2	49	0	51	2	50	2050.6374	2050.63822	-0.0008
43	1	50	1	49	0	51	1	50	2050.6533	2050.65311	0.0002
44	1	49	4	45	0	50	4	46	2050.6918	2050.69122	0.0006
45	1	47	7	40	0	48	7	41	2050.7092	2050.70969	-0.0005
46	1	46	8	38	0	47	8	39	2050.7394	2050.73959	-0.0002
47	1	49	0	49	0	50	0	50	2050.8983	2050.89813	0.0002
48	1	48	2	46	0	49	2	47	2051.0179	2051.01758	0.0003
49	1	46	4	42	0	47	4	43	2051.2912	2051.29134	-0.0001
50	1	41	8	33	0	42	8	34	2051.7573	2051.75744	-0.0001
51	1	41	8	33	0	42	8	34	2051.758	2051.75744	0.0006
52	1	44	1	43	0	45	1	44	2051.8487	2051.84908	-0.0004
53	1	43	4	39	0	44	4	40	2051.8997	2051.89949	0.0002
54	1	42	5	37	0	43	5	38	2051.9991	2051.99976	-0.0007
55	1	42	2	40	0	43	2	41	2052.2287	2052.22797	0.0007
56	1	41	0	41	0	42	0	42	2052.5227	2052.52225	0.0004
57	1	40	3	38	0	41	3	39	2052.5973	2052.59705	0.0002
58	1	39	3	37	0	40	3	38	2052.8045	2052.80419	0.0003
59	1	39	0	39	0	40	0	40	2052.9354	2052.93551	-0.0001
60	1	38	3	35	0	39	3	36	2053.01	2053.01059	-0.0006
61	1	36	5	31	0	37	5	32	2053.2449	2053.24528	-0.0004
62	1	36	4	32	0	37	4	33	2053.3494	2053.34963	-0.0002
63	1	36	3	34	0	37	3	35	2053.4308	2053.43095	-0.0001
64	1	35	5	30	0	36	5	31	2053.4554	2053.45597	-0.0006
65	1	34	3	31	0	35	3	32	2053.852	2053.85206	-0.0001
66	1	14	10	4	0	14	10	5	2060.8643	2060.86474	-0.0004
67	1	15	10	5	0	15	10	6	2060.8777	2060.87747	0.0002
68	1	16	9	7	0	16	9	8	2061.1026	2061.10222	0.0004
69	1	11	8	3	0	11	8	4	2061.2338	2061.23401	-0.0002
70	1	7	7	0	0	7	7	1	2061.3726	2061.37211	0.0005
71	1	12	7	5	0	12	7	6	2061.4148	2061.41434	0.0005
72	1	12	6	6	0	12	6	7	2061.563	2061.56305	0
73	1	9	5	4	0	9	5	5	2061.6621	2061.66196	0.0001
74	1	10	5	5	0	10	5	6	2061.6701	2061.67038	-0.0003
75	1	13	3	10	0	12	3	9	2065.0308	2065.03095	-0.0001
76	1	15	1	15	0	14	1	14	2065.5799	2065.57993	0
77	1	15	0	15	0	14	0	14	2065.6375	2065.6373	0.0002
78	1	15	1	14	0	14	1	13	2065.6795	2065.67969	-0.0002
79	1	16	0	16	0	15	0	15	2065.8911	2065.89104	0.0001
80	1	16	1	15	0	15	1	14	2065.939	2065.93838	0.0006
81	1	17	1	17	0	16	1	16	2066.0826	2066.08201	0.0006
82	1	17	2	16	0	16	2	15	2066.106	2066.10579	0.0002
83	1	18	4	14	0	17	4	13	2066.2252	2066.22556	-0.0004
84	1	19	5	14	0	18	5	13	2066.38	2066.37939	0.0006
85	1	20	4	16	0	19	4	15	2066.7423	2066.74159	0.0007
86	1	20	1	19	0	19	1	18	2066.9813	2066.98133	0



87	1	21	4	17	0	20	4	16	2067.0009	2067.00081	0.0001
88	1	21	1	21	0	20	1	20	2067.0945	2067.09403	0.0005
89	1	22	3	19	0	21	3	18	2067.3431	2067.34288	0.0002
90	1	23	1	23	0	22	1	22	2067.6044	2067.60387	0.0005
91	1	23	0	23	0	22	0	22	2067.6838	2067.68314	0.0007
92	1	27	3	24	0	26	3	23	2068.6565	2068.65609	0.0004
93	1	27	0	27	0	26	0	26	2068.7179	2068.71811	-0.0002
94	1	29	0	29	0	28	0	28	2069.2383	2069.23814	0.0002
95	1	29	2	27	0	28	2	26	2069.2754	2069.27582	-0.0004
96	1	32	7	25	0	31	7	24	2069.5272	2069.52725	0
97	1	30	2	28	0	29	2	27	2069.5457	2069.54592	-0.0002
98	1	30	1	29	0	29	1	28	2069.643	2069.64257	0.0004
99	1	31	2	30	0	30	2	29	2069.7599	2069.76048	-0.0006
100	1	35	1	35	0	34	1	34	2070.7125	2070.71292	-0.0004
101	1	36	6	30	0	35	6	29	2070.7528	2070.7527	0.0001
102	1	37	6	31	0	36	6	30	2071.0246	2071.02417	0.0004
103	1	36	0	36	0	35	0	35	2071.0694	2071.06987	-0.0005
104	1	36	3	33	0	35	3	32	2071.0726	2071.07202	0.0006
105	1	39	8	31	0	38	8	30	2071.2545	2071.25504	-0.0005
106	1	37	1	36	0	36	1	35	2071.5459	2071.54634	-0.0004
107	1	38	2	37	0	37	2	36	2071.6374	2071.63738	0
108	1	38	1	37	0	37	1	36	2071.8212	2071.82072	0.0005
109	1	39	3	37	0	38	3	36	2071.8841	2071.88369	0.0004
110	1	41	7	34	0	40	7	33	2071.9705	2071.97056	-0.0001
111	1	40	2	39	0	39	2	38	2072.1787	2072.17915	-0.0004
112	1	40	1	39	0	39	1	38	2072.3713	2072.37113	0.0002
113	1	41	0	41	0	40	0	40	2072.3879	2072.3884	-0.0005
114	1	44	8	36	0	43	8	35	2072.6304	2072.63078	-0.0004
115	1	42	3	39	0	41	3	38	2072.7202	2072.72057	-0.0004
116	1	43	1	43	0	42	1	42	2072.8297	2072.82927	0.0004
117	1	43	2	42	0	42	2	41	2072.9955	2072.99613	-0.0006
118	1	45	7	38	0	44	7	37	2073.075	2073.07515	-0.0002
119	1	43	2	41	0	42	2	40	2073.1482	2073.14848	-0.0003
120	1	43	1	42	0	42	1	41	2073.2008	2073.2006	0.0002
121	1	45	1	45	0	44	1	44	2073.3636	2073.36333	0.0003
122	1	45	3	43	0	44	3	42	2073.5376	2073.5379	-0.0003
123	1	45	1	44	0	44	1	43	2073.7563	2073.75593	0.0004
124	1	46	3	43	0	45	3	42	2073.8376	2073.83692	0.0007
125	1	47	1	47	0	46	1	46	2073.899	2073.89929	-0.0003
126	1	46	1	45	0	45	1	44	2074.0349	2074.03425	0.0006
127	1	48	0	48	0	47	0	47	2074.2486	2074.24857	0
128	1	48	4	44	0	47	4	43	2074.2931	2074.29297	0.0001
129	1	48	1	47	0	47	1	46	2074.592	2074.59208	-0.0001
130	1	49	3	47	0	48	3	46	2074.6543	2074.65445	-0.0001
131	1	53	4	49	0	52	4	48	2075.7037	2075.70323	0.0005

132	1	55	4	51	0	54	4	50	2076.2727	2076.27239	0.0003
133	1	57	6	51	0	56	6	50	2076.6011	2076.60136	-0.0003
134	1	62	6	56	0	61	6	55	2078.0368	2078.03716	-0.0004

B.12  $^{79}\text{BrNO } 2\nu_1 - \nu_3$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu'$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	62	8	54	0	63	8	55	3273.6981	3273.69821	-0.0001
2	1	61	8	53	0	62	8	54	3273.7504	3273.75026	0.0001
3	1	57	8	49	0	58	8	50	3273.99084	3273.99052	0.0003
4	1	54	8	46	0	55	8	47	3274.20356	3274.20352	0
5	1	54	8	46	0	55	8	47	3274.20352	3274.20425	-0.0007
6	1	63	7	56	0	64	7	57	3274.69452	3274.69499	-0.0005
7	1	62	7	55	0	63	7	56	3274.74336	3274.74254	0.0008
8	1	61	7	54	0	62	7	55	3274.79539	3274.79509	0.0003
9	1	46	8	38	0	47	8	39	3274.90791	3274.90813	-0.0002
10	1	58	7	51	0	59	7	52	3274.97018	3274.96954	0.0006
11	1	54	7	47	0	55	7	48	3275.2469	3275.24617	0.0007
12	1	42	8	34	0	43	8	35	3275.33462	3275.3346	0
13	1	40	8	32	0	41	8	33	3275.56659	3275.56714	-0.0006
14	1	38	8	30	0	39	8	31	3275.81098	3275.81111	-0.0001
15	1	60	5	55	0	61	5	56	3276.52939	3276.52995	-0.0006
16	1	69	4	66	0	70	4	67	3276.7853	3276.7851	0.0002
17	1	69	4	65	0	70	4	66	3276.79144	3276.79095	0.0005
18	1	67	4	63	0	68	4	64	3276.85175	3276.85146	0.0003
19	1	65	4	62	0	66	4	63	3276.9214	3276.92118	0.0002
20	1	63	4	59	0	64	4	60	3277.01106	3277.01055	0.0005
21	1	52	5	47	0	53	5	48	3277.07911	3277.07948	-0.0004
22	1	61	4	58	0	62	4	59	3277.10739	3277.10678	0.0006
23	1	61	4	57	0	62	4	58	3277.10953	3277.10883	0.0007
24	1	60	4	57	0	61	4	58	3277.16183	3277.16234	-0.0005
25	1	65	3	62	0	66	3	63	3277.44229	3277.44203	0.0003
26	1	63	3	60	0	64	3	61	3277.52368	3277.52358	0.0001
27	1	61	3	58	0	62	3	59	3277.61841	3277.61802	0.0004
28	1	46	5	41	0	47	5	42	3277.6228	3277.62295	-0.0001
29	1	60	3	57	0	61	3	58	3277.67045	3277.67025	0.0002
30	1	66	2	65	0	67	2	66	3277.68779	3277.688	-0.0002
31	1	68	2	66	0	69	2	67	3277.69553	3277.69598	-0.0005
32	1	52	4	49	0	53	4	50	3277.70967	3277.7103	-0.0006
33	1	52	4	48	0	53	4	49	3277.70994	3277.70944	0.0005
34	1	65	2	64	0	66	2	65	3277.72942	3277.72894	0.0005
35	1	69	1	68	0	70	1	69	3277.75504	3277.75478	0.0003
36	1	66	2	64	0	67	2	65	3277.76064	3277.76046	0.0002
37	1	69	1	69	0	70	1	70	3277.78573	3277.78509	0.0006

38	1	65	2	63	0	66	2	64	3277.79774	3277.7971	0.0006
39	1	68	1	68	0	69	1	69	3277.82015	3277.82078	-0.0006
40	1	63	2	62	0	64	2	63	3277.82149	3277.82112	0.0004
41	1	64	2	62	0	65	2	63	3277.83803	3277.83763	0.0004
42	1	63	2	61	0	64	2	62	3277.88126	3277.88135	-0.0001
43	1	66	1	66	0	67	1	67	3277.8978	3277.8981	-0.0003
44	1	66	0	66	0	67	0	67	3277.92022	3277.92079	-0.0006
45	1	61	2	60	0	62	2	61	3277.92556	3277.92512	0.0004
46	1	65	0	65	0	66	0	66	3277.96425	3277.96381	0.0004
47	1	49	4	45	0	50	4	46	3277.96701	3277.96683	0.0002
48	1	61	2	59	0	62	2	60	3277.97706	3277.97625	0.0008
49	1	60	2	59	0	61	2	60	3277.98213	3277.98252	-0.0004
50	1	63	1	62	0	64	1	63	3278.00161	3278.00193	-0.0003
51	1	64	0	64	0	65	0	65	3278.01148	3278.01121	0.0003
52	1	36	6	30	0	37	6	31	3278.01199	3278.01175	0.0002
53	1	60	2	58	0	61	2	59	3278.02936	3278.03019	-0.0008
54	1	63	1	63	0	64	1	64	3278.03683	3278.03756	-0.0007
55	1	59	2	58	0	60	2	59	3278.04164	3278.04109	0.0005
56	1	42	5	37	0	43	5	38	3278.04778	3278.04859	-0.0008
57	1	63	0	63	0	64	0	64	3278.06165	3278.06237	-0.0007
58	1	59	2	57	0	60	2	58	3278.08487	3278.0841	0.0008
59	1	53	3	51	0	54	3	52	3278.11956	3278.12008	-0.0005
60	1	53	3	50	0	54	3	51	3278.12783	3278.12739	0.0004
61	1	35	6	29	0	36	6	30	3278.14478	3278.14473	0.0001
62	1	60	1	59	0	61	1	60	3278.16359	3278.16314	0.0005
63	1	60	1	60	0	61	1	61	3278.20282	3278.20299	-0.0002
64	1	59	1	58	0	60	1	59	3278.22336	3278.22308	0.0003
65	1	60	0	60	0	61	0	61	3278.2303	3278.23067	-0.0004
66	1	46	4	42	0	47	4	43	3278.25218	3278.25201	0.0002
67	1	59	1	59	0	60	1	60	3278.26419	3278.26433	-0.0001
68	1	34	6	28	0	35	6	29	3278.28067	3278.28129	-0.0006
69	1	59	0	59	0	60	0	60	3278.29248	3278.29324	-0.0008
70	1	49	3	46	0	50	3	47	3278.46033	3278.45965	0.0007
71	1	38	5	33	0	39	5	34	3278.52224	3278.52235	-0.0001
72	1	43	4	39	0	44	4	40	3278.56573	3278.56563	0.0001
73	1	54	1	53	0	55	1	54	3278.56573	3278.56517	0.0006
74	1	54	1	54	0	55	1	55	3278.61563	3278.61566	0
75	1	42	4	38	0	43	4	39	3278.67648	3278.67729	-0.0008
76	1	53	0	53	0	54	0	54	3278.72771	3278.7274	0.0003
77	1	46	3	44	0	47	3	45	3278.74159	3278.74198	-0.0004
78	1	46	3	43	0	47	3	44	3278.74372	3278.74426	-0.0005
79	1	36	5	31	0	37	5	32	3278.77838	3278.77763	0.0008
80	1	41	4	37	0	42	4	38	3278.79016	3278.78983	0.0003
81	1	49	2	48	0	50	2	49	3278.80323	3278.80363	-0.0004
82	1	49	2	47	0	50	2	48	3278.81284	3278.81341	-0.0006

83	1	51	1	51	0	52	1	52	3278.86247	3278.86249	0
84	1	51	0	51	0	52	0	52	3278.89663	3278.89692	-0.0003
85	1	35	5	30	0	36	5	31	3278.91106	3278.91058	0.0005
86	1	50	1	50	0	51	1	51	3278.95053	3278.9512	-0.0007
87	1	49	1	48	0	50	1	49	3278.98202	3278.9819	0.0001
88	1	50	0	50	0	51	0	51	3278.98549	3278.98598	-0.0005
89	1	47	2	46	0	48	2	47	3278.9919	3278.99132	0.0006
90	1	49	1	49	0	50	1	50	3279.0418	3279.04245	-0.0006
91	1	34	5	29	0	35	5	30	3279.04684	3279.04752	-0.0007
92	1	43	3	41	0	44	3	42	3279.05487	3279.05568	-0.0008
93	1	49	0	49	0	50	0	50	3279.07729	3279.07694	0.0004
94	1	46	2	44	0	47	2	45	3279.0933	3279.09314	0.0002
95	1	38	4	34	0	39	4	35	3279.15067	3279.15074	-0.0001
96	1	42	3	39	0	43	3	40	3279.16615	3279.16615	0
97	1	47	1	46	0	48	1	47	3279.16962	3279.16907	0.0006
98	1	33	5	28	0	34	5	29	3279.18574	3279.18634	-0.0006
99	1	47	1	47	0	48	1	48	3279.23313	3279.23389	-0.0008
100	1	41	3	39	0	42	3	40	3279.27956	3279.27945	0.0001
101	1	41	3	38	0	42	3	39	3279.27983	3279.27947	0.0004
102	1	46	0	46	0	47	0	47	3279.37002	3279.36973	0.0003
103	1	40	3	38	0	41	3	39	3279.39644	3279.39709	-0.0006
104	1	40	3	37	0	41	3	38	3279.39644	3279.3972	-0.0008
105	1	43	2	42	0	44	2	43	3279.40605	3279.40674	-0.0007
106	1	36	4	32	0	37	4	33	3279.40632	3279.40634	0
107	1	42	2	40	0	43	2	41	3279.51226	3279.5115	0.0008
108	1	42	2	41	0	43	2	42	3279.51706	3279.51786	-0.0008
109	1	41	2	39	0	42	2	40	3279.62513	3279.62464	0.0005
110	1	41	2	40	0	42	2	41	3279.63127	3279.63193	-0.0007
111	1	43	0	43	0	44	0	44	3279.68944	3279.68913	0.0003
112	1	40	2	39	0	41	2	40	3279.74869	3279.74794	0.0007
113	1	42	1	42	0	43	1	43	3279.7639	3279.76368	0.0002
114	1	42	0	42	0	43	0	43	3279.80179	3279.80229	-0.0005
115	1	41	1	40	0	42	1	41	3279.80499	3279.80462	0.0004
116	1	41	1	41	0	42	1	42	3279.87889	3279.87833	0.0006
117	1	36	3	33	0	37	3	34	3279.89492	3279.89454	0.0004
118	1	41	0	41	0	42	0	42	3279.91707	3279.91673	0.0003
119	1	40	1	40	0	41	1	41	3279.99686	3279.99732	-0.0005
120	1	34	3	31	0	35	3	32	3280.16299	3280.16344	-0.0005
121	1	34	3	32	0	35	3	33	3280.16342	3280.16374	-0.0003
122	1	33	3	31	0	34	3	32	3280.30216	3280.30184	0.0003
123	1	10	10	0	0	10	10	1	3280.73311	3280.73373	-0.0006
124	1	10	10	0	0	10	10	1	3280.7331	3280.7331	0
125	1	12	10	2	0	12	10	3	3280.80301	3280.80354	-0.0005
126	1	13	10	3	0	13	10	4	3280.84238	3280.84222	0.0002
127	1	13	10	3	0	13	10	4	3280.84251	3280.84235	0.0002

128	1	14	10	4	0	14	10	5	3280.88487	3280.88567	-0.0008
129	1	15	10	5	0	15	10	6	3280.93039	3280.92989	0.0005
130	1	15	10	5	0	15	10	6	3280.9303	3280.93072	-0.0004
131	1	9	9	0	0	9	9	1	3282.00837	3282.00769	0.0007
132	1	10	9	1	0	10	9	2	3282.03875	3282.03917	-0.0004
133	1	12	9	3	0	12	9	4	3282.10863	3282.10906	-0.0004
134	1	13	9	4	0	13	9	5	3282.14812	3282.1483	-0.0002
135	1	14	9	5	0	14	9	6	3282.19065	3282.1909	-0.0003
136	1	16	9	7	0	16	9	8	3282.28481	3282.28462	0.0002
137	1	10	8	2	0	10	8	3	3283.21073	3283.21079	-0.0001
138	1	13	8	5	0	13	8	6	3283.32019	3283.32095	-0.0008
139	1	14	8	6	0	14	8	7	3283.36275	3283.36278	0
140	1	15	8	7	0	15	8	8	3283.40835	3283.40778	0.0006
141	1	7	7	0	0	7	7	1	3284.16561	3284.16536	0.0003
142	1	8	7	1	0	8	7	2	3284.18996	3284.19063	-0.0007
143	1	10	7	3	0	10	7	4	3284.24777	3284.24742	0.0003
144	1	12	7	5	0	12	7	6	3284.31776	3284.31844	-0.0007
145	1	7	6	1	0	7	6	2	3285.06657	3285.06578	0.0008
146	1	8	6	2	0	8	6	3	3285.09093	3285.0905	0.0004
147	1	10	6	4	0	10	6	5	3285.14879	3285.14903	-0.0002
148	1	5	5	0	0	5	5	1	3285.79094	3285.79029	0.0006
149	1	8	5	3	0	8	5	4	3285.85492	3285.85436	0.0006
150	1	11	5	6	0	11	5	7	3285.94632	3285.94602	0.0003
151	1	4	4	0	0	4	4	1	3286.40186	3286.4019	0
152	1	5	4	1	0	5	4	2	3286.4171	3286.41719	-0.0001
153	1	6	4	2	0	6	4	3	3286.43539	3286.43571	-0.0003
154	1	7	4	3	0	7	4	4	3286.45672	3286.45678	-0.0001
155	1	8	4	4	0	8	4	5	3286.48111	3286.48095	0.0002
156	1	10	4	6	0	10	4	7	3286.53902	3286.53844	0.0006
157	1	11	4	7	0	10	4	6	3289.25088	3289.25158	-0.0007
158	1	14	4	10	0	13	4	9	3290.09991	3290.10017	-0.0003
159	1	13	3	10	0	12	3	9	3290.30154	3290.30126	0.0003
160	1	15	4	11	0	14	4	10	3290.38897	3290.38964	-0.0007
161	1	14	3	11	0	13	3	10	3290.58763	3290.58711	0.0005
162	1	17	4	13	0	16	4	12	3290.97615	3290.97618	0
163	1	18	4	14	0	17	4	13	3291.27427	3291.2741	0.0002
164	1	15	1	15	0	14	1	14	3291.38134	3291.38125	0.0001
165	1	15	1	14	0	14	1	13	3291.48298	3291.48291	0.0001
166	1	21	5	16	0	20	5	15	3291.56059	3291.56059	0
167	1	18	3	15	0	17	3	14	3291.76238	3291.76279	-0.0004
168	1	16	1	15	0	15	1	14	3291.77865	3291.77842	0.0002
169	1	16	0	16	0	15	0	15	3291.78783	3291.78798	-0.0001
170	1	17	2	16	0	16	2	15	3291.80983	3291.80922	0.0006
171	1	22	5	17	0	21	5	16	3291.87067	3291.87072	-0.0001
172	1	17	1	17	0	16	1	16	3291.95926	3291.9585	0.0008

173	1	17	0	17	0	16	0	16	3292.08113	3292.08095	0.0002
174	1	31	8	23	0	30	8	22	3292.09456	3292.09402	0.0005
175	1	21	4	17	0	20	4	16	3292.18662	3292.18594	0.0007
176	1	18	0	18	0	17	0	17	3292.37721	3292.37774	-0.0005
177	1	22	4	18	0	21	4	17	3292.49697	3292.49623	0.0007
178	1	19	1	19	0	18	1	18	3292.54864	3292.54818	0.0005
179	1	19	1	18	0	18	1	17	3292.68381	3292.68402	-0.0002
180	1	23	4	19	0	22	4	18	3292.80999	3292.81057	-0.0006
181	1	34	8	26	0	33	8	25	3293.12274	3293.12281	-0.0001
182	1	31	7	24	0	30	7	23	3293.13128	3293.1309	0.0004
183	1	22	1	22	0	21	1	21	3293.45407	3293.45332	0.0007
184	1	27	5	22	0	26	5	21	3293.46618	3293.46673	-0.0006
185	1	22	0	22	0	21	0	21	3293.58876	3293.58949	-0.0007
186	1	22	1	21	0	21	1	20	3293.61599	3293.61607	-0.0001
187	1	23	2	22	0	22	2	21	3293.64016	3293.63958	0.0006
188	1	23	2	21	0	22	2	20	3293.66471	3293.66394	0.0008
189	1	23	1	23	0	22	1	22	3293.76156	3293.76162	-0.0001
190	1	36	8	28	0	35	8	27	3293.82296	3293.82265	0.0003
191	1	23	0	23	0	22	0	22	3293.89835	3293.89836	0
192	1	23	1	22	0	22	1	21	3293.93266	3293.9324	0.0003
193	1	27	4	23	0	26	4	22	3294.09301	3294.09294	0.0001
194	1	29	5	24	0	28	5	23	3294.1253	3294.12511	0.0002
195	1	34	7	27	0	33	7	26	3294.15945	3294.15875	0.0007
196	1	37	8	29	0	36	8	28	3294.1776	3294.17759	0
197	1	25	2	24	0	24	2	23	3294.27355	3294.27416	-0.0006
198	1	30	5	25	0	29	5	24	3294.4594	3294.4593	0.0001
199	1	25	0	25	0	24	0	24	3294.52544	3294.52477	0.0007
200	1	38	8	30	0	37	8	29	3294.53491	3294.5345	0.0004
201	1	36	7	29	0	35	7	28	3294.85994	3294.86053	-0.0006
202	1	30	4	26	0	29	4	25	3295.08657	3295.08617	0.0004
203	1	37	7	30	0	36	7	29	3295.21458	3295.21536	-0.0008
204	1	31	4	27	0	30	4	26	3295.42378	3295.42377	0
205	1	38	7	31	0	37	7	30	3295.5719	3295.57269	-0.0008
206	1	41	8	33	0	40	8	32	3295.625	3295.6252	-0.0002
207	1	34	5	29	0	33	5	28	3295.82514	3295.82515	0
208	1	30	2	29	0	29	2	28	3295.90808	3295.90794	0.0001
209	1	31	3	28	0	30	3	27	3295.91667	3295.9172	-0.0005
210	1	30	2	28	0	29	2	27	3295.96664	3295.96669	-0.0001
211	1	30	1	30	0	29	1	29	3295.99269	3295.99334	-0.0006
212	1	42	8	34	0	41	8	33	3295.99406	3295.99455	-0.0005
213	1	30	0	30	0	29	0	29	3296.13847	3296.13902	-0.0006
214	1	31	2	30	0	30	2	29	3296.24356	3296.24279	0.0008
215	1	31	2	29	0	30	2	28	3296.30865	3296.30783	0.0008
216	1	31	0	31	0	30	0	30	3296.46872	3296.46882	-0.0001
217	1	31	1	30	0	30	1	29	3296.57137	3296.57143	-0.0001

218	1	32	1	32	0	31	1	31	3296.65527	3296.65448	0.0008
219	1	41	7	34	0	40	7	33	3296.66225	3296.66203	0.0002
220	1	35	4	31	0	34	4	30	3296.80262	3296.8031	-0.0005
221	1	42	7	35	0	41	7	34	3297.03158	3297.03199	-0.0004
222	1	36	4	32	0	35	4	31	3297.15475	3297.1553	-0.0005
223	1	38	5	33	0	37	5	32	3297.23865	3297.23937	-0.0007
224	1	46	8	38	0	45	8	37	3297.4999	3297.50003	-0.0001
225	1	37	4	33	0	36	4	32	3297.50991	3297.5092	0.0007
226	1	44	7	37	0	43	7	36	3297.77876	3297.77953	-0.0008
227	1	38	4	34	0	37	4	33	3297.86815	3297.86833	-0.0002
228	1	36	2	35	0	35	2	34	3297.96408	3297.96427	-0.0002
229	1	36	1	36	0	35	1	35	3298.01363	3298.01354	0.0001
230	1	36	0	36	0	35	0	35	3298.15768	3298.15833	-0.0007
231	1	37	0	37	0	36	0	36	3298.50299	3298.50273	0.0003
232	1	40	4	36	0	39	4	35	3298.59319	3298.59342	-0.0002
233	1	37	1	36	0	36	1	35	3298.67017	3298.66989	0.0003
234	1	38	1	38	0	37	1	37	3298.70927	3298.70959	-0.0003
235	1	38	0	38	0	37	0	37	3298.8508	3298.85013	0.0007
236	1	47	7	40	0	46	7	39	3298.92168	3298.92251	-0.0008
237	1	41	4	37	0	40	4	36	3298.96038	3298.9601	0.0003
238	1	38	1	37	0	37	1	36	3299.02966	3299.02994	-0.0003
239	1	40	3	38	0	39	3	37	3299.0842	3299.08403	0.0002
240	1	42	4	38	0	41	4	37	3299.3305	3299.33054	0
241	1	41	3	39	0	40	3	38	3299.45112	3299.4507	0.0004
242	1	41	3	38	0	40	3	37	3299.46526	3299.46471	0.0005
243	1	40	0	40	0	39	0	39	3299.55395	3299.55462	-0.0007
244	1	41	2	40	0	40	2	39	3299.75502	3299.75579	-0.0008
245	1	40	1	39	0	39	1	38	3299.75676	3299.75596	0.0008
246	1	41	1	41	0	40	1	40	3299.77347	3299.7731	0.0004
247	1	42	3	39	0	41	3	38	3299.83725	3299.83698	0.0003
248	1	41	2	39	0	40	2	38	3299.90828	3299.90896	-0.0007
249	1	44	4	40	0	43	4	39	3300.07955	3300.07914	0.0004
250	1	41	1	40	0	40	1	39	3300.12434	3300.12371	0.0006
251	1	42	1	42	0	41	1	41	3300.13345	3300.13329	0.0002
252	1	42	0	42	0	41	0	41	3300.2672	3300.26724	0
253	1	42	2	40	0	41	2	39	3300.28589	3300.28581	0.0001
254	1	42	1	41	0	41	1	40	3300.49457	3300.49397	0.0006
255	1	44	3	42	0	43	3	41	3300.57002	3300.57076	-0.0007
256	1	44	3	41	0	43	3	40	3300.59057	3300.59108	-0.0005
257	1	44	2	43	0	43	2	42	3300.86303	3300.86328	-0.0003
258	1	44	0	44	0	43	0	43	3300.9906	3300.99096	-0.0004
259	1	44	2	42	0	43	2	41	3301.05046	3301.04966	0.0008
260	1	47	4	43	0	46	4	42	3301.22568	3301.22615	-0.0005
261	1	44	1	43	0	43	1	42	3301.24293	3301.24232	0.0006
262	1	46	3	44	0	45	3	43	3301.33055	3301.33031	0.0002

263	1	48	4	44	0	47	4	43	3301.61368	3301.61385	-0.0002
264	1	47	3	45	0	46	3	44	3301.71507	3301.71576	-0.0007
265	1	47	3	44	0	46	3	43	3301.74424	3301.74478	-0.0005
266	1	47	2	46	0	46	2	45	3301.99566	3301.9951	0.0006
267	1	47	0	47	0	46	0	46	3302.09497	3302.09547	-0.0005
268	1	48	3	45	0	47	3	44	3302.13511	3302.13536	-0.0003
269	1	47	2	45	0	46	2	44	3302.2203	3302.22048	-0.0002
270	1	47	1	46	0	46	1	45	3302.38484	3302.38468	0.0002
271	1	50	4	46	0	49	4	45	3302.39849	3302.39831	0.0002
272	1	48	0	48	0	47	0	47	3302.4684	3302.46785	0.0006
273	1	48	1	47	0	47	1	46	3302.77056	3302.77065	-0.0001
274	1	51	4	47	0	50	4	46	3302.7953	3302.79584	-0.0005
275	1	55	6	49	0	54	6	48	3303.00157	3303.00083	0.0007
276	1	51	3	48	0	50	3	47	3303.32696	3303.3267	0.0003
277	1	54	4	51	0	53	4	50	3304.00038	3304.00005	0.0003
278	1	54	4	50	0	53	4	49	3304.00383	3304.0044	-0.0006



B.13  $^{81}\text{BrNO } 2\nu_1 - \nu_3$

N	$\nu'$	$J'$	$K'_a$	$K'_c$	$\nu'$	$J''$	$K''_a$	$K''_c$	Obs	Pred	Diff
1	1	62	8	54	0	63	8	55	3273.5811	3273.580643	0.0005
2	1	62	8	54	0	63	8	55	3273.5812	3273.580896	0.0003
3	1	61	8	53	0	62	8	54	3273.6329	3273.633046	-0.0002
4	1	61	8	53	0	62	8	54	3273.633	3273.633738	-0.0007
5	1	58	8	50	0	59	8	51	3273.8067	3273.807022	-0.0004
6	1	58	8	50	0	59	8	51	3273.8067	3273.806795	-0.0001
7	1	57	8	49	0	58	8	50	3273.8708	3273.871168	-0.0004
8	1	54	8	46	0	55	8	47	3274.0817	3274.081863	-0.0002
9	1	54	8	46	0	55	8	47	3274.0816	3274.081898	-0.0003
10	1	53	8	45	0	54	8	46	3274.1581	3274.15804	0.0001
11	1	63	7	56	0	64	7	57	3274.5739	3274.573152	0.0008
12	1	63	7	56	0	64	7	57	3274.5739	3274.573735	0.0002
13	1	62	7	55	0	63	7	56	3274.6225	3274.622075	0.0004
14	1	61	7	54	0	62	7	55	3274.674	3274.674332	-0.0004
15	1	46	8	38	0	47	8	39	3274.78	3274.779419	0.0006
16	1	58	7	51	0	59	7	52	3274.8472	3274.847562	-0.0004
17	1	58	7	51	0	59	7	52	3274.8472	3274.847481	-0.0003
18	1	54	7	47	0	55	7	48	3275.1212	3275.121621	-0.0004
19	1	42	8	34	0	43	8	35	3275.2033	3275.202751	0.0005
20	1	42	8	34	0	43	8	35	3275.2034	3275.203139	0.0003
21	1	40	8	32	0	41	8	33	3275.4335	3275.433918	-0.0005
22	1	40	8	32	0	41	8	33	3275.4334	3275.43323	0.0002
23	1	38	8	30	0	39	8	31	3275.676	3275.675975	0
24	1	60	5	55	0	61	5	56	3276.4016	3276.40231	-0.0007
25	1	69	4	66	0	70	4	67	3276.6596	3276.658976	0.0006
26	1	69	4	65	0	70	4	66	3276.6655	3276.66597	-0.0005
27	1	68	4	64	0	69	4	65	3276.6938	3276.693422	0.0003
28	1	54	5	49	0	55	5	50	3276.7912	3276.790635	0.0005
29	1	65	4	62	0	66	4	63	3276.7938	3276.793531	0.0003
30	1	65	4	61	0	66	4	62	3276.7973	3276.797928	-0.0006
31	1	53	5	48	0	54	5	49	3276.8672	3276.866831	0.0004
32	1	63	4	60	0	64	4	61	3276.8798	3276.880515	-0.0007
33	1	63	4	59	0	64	4	60	3276.8824	3276.882207	0.0002
34	1	52	5	47	0	53	5	48	3276.9462	3276.946462	-0.0003
35	1	61	4	57	0	62	4	58	3276.9801	3276.980856	-0.0008
36	1	60	4	56	0	61	4	57	3277.0335	3277.033045	0.0004
37	1	49	5	44	0	50	5	45	3277.2017	3277.202054	-0.0004
38	1	66	3	63	0	67	3	64	3277.2782	3277.277972	0.0002
39	1	65	3	62	0	66	3	63	3277.3137	3277.313637	0
40	1	63	3	60	0	64	3	61	3277.394	3277.393338	0.0007
41	1	61	3	59	0	62	3	60	3277.4639	3277.46393	0

42	1	46	5	41	0	47	5	42	3277.4852	3277.485932	-0.0007
43	1	61	3	58	0	62	3	59	3277.4877	3277.487418	0.0002
44	1	60	3	58	0	61	3	59	3277.5181	3277.518487	-0.0004
45	1	60	3	57	0	61	3	58	3277.5392	3277.539749	-0.0006
46	1	66	2	65	0	67	2	66	3277.5568	3277.557444	-0.0007
47	1	68	2	66	0	69	2	67	3277.5696	3277.569449	0.0001
48	1	52	4	48	0	53	4	49	3277.5749	3277.57544	-0.0005
49	1	69	1	69	0	70	1	70	3277.651	3277.650301	0.0007
50	1	68	1	67	0	69	1	68	3277.6619	3277.662232	-0.0003
51	1	65	2	63	0	66	2	64	3277.6705	3277.671128	-0.0007
52	1	68	1	68	0	69	1	69	3277.6849	3277.684126	0.0007
53	1	63	2	62	0	64	2	63	3277.6891	3277.688811	0.0003
54	1	63	2	61	0	64	2	62	3277.7529	3277.753176	-0.0003
55	1	66	1	66	0	67	1	67	3277.7617	3277.762094	-0.0004
56	1	65	1	64	0	66	1	65	3277.7796	3277.77904	0.0006
57	1	66	0	66	0	67	0	67	3277.7849	3277.785208	-0.0003
58	1	61	2	60	0	62	2	61	3277.7921	3277.791506	0.0006
59	1	65	1	65	0	66	1	66	3277.8047	3277.804207	0.0005
60	1	65	0	65	0	66	0	66	3277.8287	3277.828823	-0.0001
61	1	49	4	45	0	50	4	46	3277.8297	3277.829103	0.0006
62	1	61	2	59	0	62	2	60	3277.8474	3277.846947	0.0004
63	1	60	2	59	0	61	2	60	3277.8482	3277.847954	0.0002
64	1	64	1	64	0	65	1	65	3277.8506	3277.850775	-0.0002
65	1	36	6	30	0	37	6	31	3277.868	3277.86799	0
66	1	63	1	62	0	64	1	63	3277.8722	3277.871775	0.0004
67	1	64	0	64	0	65	0	65	3277.8757	3277.875057	0.0006
68	1	60	2	58	0	61	2	59	3277.8991	3277.89989	-0.0008
69	1	63	1	63	0	64	1	64	3277.8997	3277.899228	0.0004
70	1	59	2	58	0	60	2	59	3277.9071	3277.90761	-0.0005
71	1	54	3	52	0	55	3	53	3277.908	3277.908471	-0.0005
72	1	54	3	51	0	55	3	52	3277.9176	3277.918136	-0.0006
73	1	63	0	63	0	64	0	64	3277.9253	3277.925538	-0.0002
74	1	59	2	57	0	60	2	58	3277.9541	3277.95447	-0.0004
75	1	61	1	60	0	62	1	61	3277.9763	3277.97612	0.0001
76	1	53	3	51	0	54	3	52	3277.9837	3277.984254	-0.0005
77	1	35	6	29	0	36	6	30	3277.9998	3277.999323	0.0005
78	1	61	1	61	0	62	1	62	3278.0064	3278.0059	0.0005
79	1	60	1	59	0	61	1	60	3278.0326	3278.032295	0.0003
80	1	59	1	58	0	60	1	59	3278.0918	3278.091894	-0.0001
81	1	60	0	60	0	61	0	61	3278.0926	3278.092779	-0.0002
82	1	46	4	42	0	47	4	43	3278.1126	3278.113017	-0.0004
83	1	59	1	59	0	60	1	60	3278.1252	3278.12442	0.0007
84	1	34	6	28	0	35	6	29	3278.1347	3278.134233	0.0005
85	1	40	5	35	0	41	5	36	3278.1361	3278.135854	0.0002
86	1	59	0	59	0	60	0	60	3278.1543	3278.15388	0.0004

87	1	49	3	47	0	50	3	48	3278.3176	3278.318111	-0.0006
88	1	49	3	46	0	50	3	47	3278.3218	3278.322292	-0.0005
89	1	38	5	33	0	39	5	34	3278.3776	3278.377758	-0.0002
90	1	43	4	39	0	44	4	40	3278.4235	3278.422828	0.0007
91	1	54	1	54	0	55	1	55	3278.4739	3278.47453	-0.0006
92	1	54	0	54	0	55	0	55	3278.5073	3278.507155	0.0001
93	1	42	4	38	0	43	4	39	3278.5334	3278.53308	0.0004
94	1	53	1	53	0	54	1	54	3278.5527	3278.552006	0.0007
95	1	53	0	53	0	54	0	54	3278.5866	3278.585914	0.0006
96	1	46	3	44	0	47	3	45	3278.6004	3278.599885	0.0005
97	1	41	4	37	0	42	4	38	3278.6463	3278.646524	-0.0002
98	1	49	2	48	0	50	2	49	3278.6626	3278.663345	-0.0007
99	1	51	1	51	0	52	1	52	3278.7189	3278.719214	-0.0003
100	1	51	0	51	0	52	0	52	3278.7541	3278.753763	0.0004
101	1	40	4	36	0	41	4	37	3278.7624	3278.761984	0.0004
102	1	35	5	30	0	36	5	31	3278.7635	3278.764223	-0.0007
103	1	50	1	50	0	51	1	51	3278.8064	3278.806816	-0.0004
104	1	50	0	50	0	51	0	51	3278.8425	3278.842831	-0.0004
105	1	49	1	48	0	50	1	49	3278.8435	3278.843298	0.0002
106	1	47	2	46	0	48	2	47	3278.8497	3278.849034	0.0006
107	1	49	1	49	0	50	1	50	3278.8972	3278.896794	0.0004
108	1	46	2	45	0	47	2	46	3278.9479	3278.94742	0.0004
109	1	46	2	44	0	47	2	45	3278.9527	3278.952853	-0.0002
110	1	42	3	40	0	43	3	41	3279.0213	3279.021757	-0.0005
111	1	42	3	39	0	43	3	40	3279.0218	3279.021147	0.0006
112	1	47	1	46	0	48	1	47	3279.0295	3279.029799	-0.0003
113	1	33	5	28	0	34	5	29	3279.0362	3279.036305	-0.0001
114	1	47	1	47	0	48	1	48	3279.0872	3279.087016	0.0001
115	1	47	0	47	0	48	0	48	3279.1245	3279.124244	0.0003
116	1	46	1	45	0	47	1	46	3279.1269	3279.12747	-0.0005
117	1	41	3	39	0	42	3	40	3279.1341	3279.133526	0.0006
118	1	41	3	38	0	42	3	39	3279.1344	3279.134532	-0.0001
119	1	46	1	46	0	47	1	47	3279.1864	3279.187196	-0.0008
120	1	45	1	44	0	46	1	45	3279.2275	3279.227393	0.0001
121	1	40	3	37	0	41	3	38	3279.2502	3279.25019	0
122	1	36	4	32	0	37	4	33	3279.2577	3279.257275	0.0004
123	1	43	2	41	0	44	2	42	3279.2593	3279.258662	0.0006
124	1	43	2	42	0	44	2	43	3279.2606	3279.260258	0.0004
125	1	42	2	40	0	43	2	41	3279.3679	3279.367497	0.0004
126	1	42	2	41	0	43	2	42	3279.3708	3279.370394	0.0004
127	1	43	1	42	0	44	1	43	3279.4375	3279.437018	0.0005
128	1	41	2	39	0	42	2	40	3279.4797	3279.480415	-0.0007
129	1	43	1	43	0	44	1	44	3279.5027	3279.503017	-0.0004
130	1	43	0	43	0	44	0	44	3279.5416	3279.541537	0.0001
131	1	42	1	41	0	43	1	42	3279.5472	3279.546838	0.0004

132	1	42	1	42	0	43	1	43	3279.6142	3279.613588	0.0006
133	1	42	0	42	0	43	0	43	3279.6532	3279.652439	0.0007
134	1	41	1	40	0	42	1	41	3279.6598	3279.659474	0.0003
135	1	41	1	41	0	42	1	42	3279.7284	3279.728763	-0.0003
136	1	36	3	34	0	37	3	35	3279.7452	3279.744731	0.0004
137	1	41	0	41	0	42	0	42	3279.7676	3279.76795	-0.0003
138	1	40	1	39	0	41	1	40	3279.7754	3279.775586	-0.0002
139	1	40	0	40	0	41	0	41	3279.8851	3279.884891	0.0002
140	1	34	3	31	0	35	3	32	3280.011	3280.011557	-0.0006
141	1	34	3	32	0	35	3	33	3280.0113	3280.011056	0.0003
142	1	33	3	31	0	34	3	32	3280.149	3280.149101	-0.0001
143	1	10	10	0	0	10	10	1	3280.5572	3280.557725	-0.0006
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145	1	12	10	2	0	12	10	3	3280.6266	3280.625983	0.0006
146	1	12	10	2	0	12	10	3	3280.6266	3280.627166	-0.0005
147	1	13	10	3	0	13	10	4	3280.6659	3280.666303	-0.0004
148	1	13	10	3	0	13	10	4	3280.6659	3280.665359	0.0005
149	1	14	10	4	0	14	10	5	3280.7083	3280.7084	-0.0001
150	1	15	10	5	0	15	10	6	3280.7535	3280.754107	-0.0007
151	1	15	10	5	0	15	10	6	3280.7534	3280.753399	0
152	1	9	9	0	0	9	9	1	3281.8274	3281.826984	0.0004
153	1	10	9	1	0	10	9	2	3281.8577	3281.858257	-0.0006
154	1	12	9	3	0	12	9	4	3281.9272	3281.92641	0.0008
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157	1	16	9	7	0	16	9	8	3282.1025	3282.101947	0.0005
158	1	12	8	4	0	12	8	5	3283.0948	3283.095031	-0.0002
159	1	14	8	6	0	14	8	7	3283.1765	3283.176483	0
160	1	15	8	7	0	15	8	8	3283.2218	3283.221298	0.0005
161	1	7	7	0	0	7	7	1	3283.9768	3283.977018	-0.0002
162	1	8	7	1	0	8	7	2	3284.001	3284.001068	-0.0001
163	1	10	7	3	0	10	7	4	3284.0585	3284.058796	-0.0003
164	1	12	7	5	0	12	7	6	3284.1282	3284.127523	0.0006
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168	1	13	6	7	0	13	6	8	3285.0655	3285.06593	-0.0005
169	1	5	5	0	0	5	5	1	3285.5967	3285.596815	-0.0001
170	1	6	5	1	0	6	5	2	3285.6149	3285.615581	-0.0007
171	1	7	5	2	0	7	5	3	3285.6361	3285.636234	-0.0001
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177	1	7	4	3	0	7	4	4	3286.2603	3286.259584	0.0007
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179	1	15	4	11	0	14	4	10	3290.1674	3290.16729	0.0002
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192	1	16	1	15	0	15	1	14	3291.5518	3291.551569	0.0002
193	1	16	0	16	0	15	0	15	3291.5612	3291.560855	0.0003
194	1	17	2	16	0	16	2	15	3291.5822	3291.582438	-0.0002
195	1	22	5	17	0	21	5	16	3291.638	3291.637707	0.0003
196	1	17	1	17	0	16	1	16	3291.7312	3291.731035	0.0002
197	1	17	1	16	0	16	1	15	3291.8486	3291.848044	0.0006
198	1	17	0	17	0	16	0	16	3291.8527	3291.85225	0.0004
199	1	18	2	17	0	17	2	16	3291.8779	3291.878155	-0.0003
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202	1	18	0	18	0	17	0	17	3292.1469	3292.146521	0.0004
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204	1	19	2	18	0	18	2	17	3292.1768	3292.177409	-0.0007
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206	1	19	1	19	0	18	1	18	3292.3169	3292.317447	-0.0005
207	1	19	0	19	0	18	0	18	3292.4439	3292.443814	0.0001
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210	1	31	7	24	0	30	7	23	3292.8863	3292.886049	0.0003
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214	1	23	2	22	0	22	2	21	3293.4011	3293.400325	0.0007
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221	1	37	8	29	0	36	8	28	3293.9238	3293.924588	-0.0008

222	1	25	2	24	0	24	2	23	3294.0306	3294.030911	-0.0003
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224	1	30	5	25	0	29	5	24	3294.211	3294.21119	-0.0002
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257	1	47	8	39	0	46	8	38	3297.6077	3297.606972	0.0007
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261	1	37	1	37	0	36	1	36	3298.0923	3298.092183	0.0001
262	1	37	0	37	0	36	0	36	3298.2359	3298.236094	-0.0002
263	1	37	1	36	0	36	1	35	3298.402	3298.402712	-0.0007
264	1	42	5	37	0	41	5	36	3298.4253	3298.425961	-0.0006
265	1	41	4	37	0	40	4	36	3298.6863	3298.686896	-0.0006
266	1	38	1	37	0	37	1	36	3298.7594	3298.760028	-0.0006

267	1	42	4	38	0	41	4	37	3299.054	3299.054727	-0.0007
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271	1	41	2	40	0	40	2	39	3299.4789	3299.479233	-0.0003
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277	1	42	0	42	0	41	0	41	3299.9896	3299.989946	-0.0003
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280	1	44	3	42	0	43	3	41	3300.2877	3300.287641	0
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282	1	44	1	44	0	43	1	43	3300.5789	3300.578618	0.0003
283	1	44	2	43	0	43	2	42	3300.5802	3300.580453	-0.0003
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286	1	47	4	43	0	46	4	42	3300.9377	3300.938355	-0.0006
287	1	44	1	43	0	43	1	42	3300.96	3300.960571	-0.0006
288	1	46	3	44	0	45	3	43	3301.0434	3301.04272	0.0007
289	1	48	4	44	0	47	4	43	3301.3233	3301.322873	0.0005
290	1	47	3	45	0	46	3	44	3301.4259	3301.425375	0.0005
291	1	47	3	44	0	46	3	43	3301.4542	3301.454691	-0.0005
292	1	47	1	47	0	46	1	46	3301.6852	3301.685472	-0.0003
293	1	47	2	46	0	46	2	45	3301.7062	3301.705882	0.0003
294	1	48	3	46	0	47	3	45	3301.8112	3301.810847	0.0003
295	1	47	2	45	0	46	2	44	3301.9284	3301.928589	-0.0002
296	1	47	1	46	0	46	1	45	3302.0954	3302.095802	-0.0004
297	1	50	4	46	0	49	4	45	3302.1036	3302.103672	-0.0001
298	1	48	0	48	0	47	0	47	3302.1775	3302.177429	0.0001
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301	1	55	6	49	0	54	6	48	3302.7	3302.700246	-0.0002
302	1	52	4	48	0	51	4	47	3302.8956	3302.895974	-0.0003
303	1	51	3	49	0	50	3	48	3302.9837	3302.983525	0.0002
304	1	54	4	51	0	53	4	50	3303.696	3303.696048	0
305	1	54	4	50	0	53	4	49	3303.6994	3303.698643	0.0007

### *Vita*

Capt Patrick E. Godfrey [REDACTED]

[REDACTED] He graduated from Clemson University in 1980 and worked in the oil industry in Louisiana and Texas for several years before joining the Air Force in 1986. His first assignment after Officer Training School was to the Air Force Weapons Laboratory at Kirtland AFB where his activities included the prediction and simulation of airblast effects from nuclear and conventional weapons. He managed the shock tube facility at Kirtland and participated in several large scale multi-national nuclear simulations. After obtaining his master's degree from AFIT in 1989 he was assigned to the Ballistic Missile Office at Norton AFB. There he managed the design, construction and flight of test vehicles and payloads based on refurbished Minuteman I and II ICBMs, in support of the Strategic Defense Initiative. He returned to AFIT in 1993 and is currently assigned to WL/AAJS at Wright-Patterson AFB. He is married to the former Wendy Hope Boelter of Wausaw, Wisconsin.



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13. ABSTRACT (Maximum 200 words) The kinetics of BrNO formation and destruction were examined using time-resolved photolysis techniques. The equilibrium constant for the dark reaction $\text{Br}_2 + 2\text{NO} \rightleftharpoons 2\text{BrNO}$ was determined as $K_{eq} = 168 \pm 23 \text{ atm}^{-1}$ and the rate constant for the forward reaction as $k_f = 1.40 \pm .18 \times 10^{-38} \text{ cm}^6/\text{molecule}^2\text{-s}$ at 293K. A novel technique for the fitting of the observed time profiles to the three-body kinetics was developed which utilizes the complete temporal profile to establish the rate coefficients. When an equilibrium mixture of Br <sub>2</sub> , NO and BrNO is disturbed by photolysis, BrNO is rapidly removed by reaction with atomic bromine. For continuous photolysis, a new photostationary condition is achieved which shifts the equilibrium toward Br <sub>2</sub> and NO. A kinetic mechanism and rates for the photolysis of such mixtures has been validated for total pressures of 28-111 torr and nitric oxide to molecular bromine concentration ratios of 2.18-26.75, with an average Br <sub>2</sub> photolysis rate of 0.050 molecules/s. The rotation structure of the $n_1 + n_2 - n_3$ , $2n_1 - n_3$ , $2n_1, 3n_1$ , $2n_1 + n_3$ and $3n_1 + n_3$ overtone and combination bands of BrNO were examined at high resolution (.005 - .01 cm <sup>-1</sup> ) using Fourier Transform Spectroscopy. Over 4900 spectral lines were recorded for the two isotopes <sup>79</sup> BrNO and <sup>81</sup> BrNO. The rotational and quartic distortion terms, inertia defects and asymmetry parameters were determined for the (200), (300), (001), (200), (301) and (110) vibrational levels. The first-order vibration-rotation interaction terms were also determined.				
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